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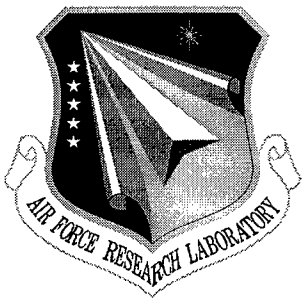

QUANTUM COMPUTING

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This report presents the derivation of quantum mechanical Hamiltonians and quantum logics as applied to the concept of quantum computation. The Hamiltonians and quantum logics derived herein are potentially realizable in spin-bearing solid state crystals or trapped ionic species. The study of quantum mechanical analogues to conventional digital computers is in its infancy and there is still much speculation regarding the eventual successful building of a quantum computer.

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Abstract

This report presents the derivation of quantum mechanical Hamiltonians and quantum logics as applied to the concept of quantum computation. The Hamiltonians and quantum logics derived herein are potentially realizable in spin-bearing solid state crystals or trapped ionic species. The study of quantum mechanical analogues to conventional digital computers is in its infancy and there is still much speculation regarding the eventual successful building of a quantum computer.

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PREFACE

Unfühlend Ist die Natur *Goethe*[1]

Science, argued Bertrand Russel deals with known facts, philosophy with speculation. However, theoretical science, especially it seems, the so-called quantum theory, is somehow an adventure comprising both. Schrödinger explains further— "The great revelation of quantum theory was that features of discreteness were discovered in the Book of Nature, in a context in which anything other than continuity seemed absurd according to the views held until then."[2]

Quantum Theory is really not a physical theory at all — certainly not in the same sense as general relativity or electromagnetics, in which all laws and knowledge can be derived from first principles. We are thus left with the unsatisfying title: Quantum Mechanics. This name is really quite precise, for like an automobile mechanic, the quantum mechanic really does not know the inner physics of each part of his apparatus, he knows how to "measure and fix"the"state"of the machinery. Max Born argued that it is quite unknowable- almost religiously. All one may "know" according to Born is that a measurement has taken place, don't ask, as Einstein and deBroglie whether or not a particle "knows" its spin, simply measure it and then go home.[3]

It is this strange world of quantum mechanics, which admits that strange things happen- such as superposition of states, that we enter when seeking to pr[illegible]m quantum computation. This world is one in which Nobel prize-winning physicists argue violently about interpretations of experiments and extrapolations of theories. Yet, it is also the very basis of our universe. The very strangeness of quantum mechanical superposition and coherence allows for formulation of new computational structures at the atomic scale. From a hardware perspective, imagine a switch(analogue to a modern day VHSIC transistor) comprised of only one atom- with quantum bit (q-bit) switching times in the fractional femtoseconds. From a software perspective, the quantum computation community has realized that the ability to store and process information at the quantum mechanical scale holds the potential to formulate and solve problems of much higher computational complexity than that of current-day supercomputers.

Information is physical in nature. This is true whether it is represented as our fingers, stones, beads on an abacus, writing on paper, voltages in a transistor circuit, or even quantum mechanical spin states of atomic species. The ability to store and manipulate the latter is referred to herein as *quantum computation*. **Quantum Computation represents, quite literally, the Quantum Limit of Information.** Quantum computation may be the vehicle to access the ultimate "fast lane"in information dominance. The old adage ,"the quick and the dead" is more applicable today than ever. Whole economies dominate or are subjugated based solely upon the speed by which they process information. "From now on, the world will be split between the fast and the slow. Historically, power has shifted from the slow to the fast[illegible]. In fast economies, advanced technology speeds production. Fast economies generate wealth faster than slow ones."[4]

As discussed in the last section, information is not an abstract entity. It is inextricably tied to a physical representation. As such it is subject to the laws of physics. This idea goes far beyond Shannon-Weiner -type theories of information, which by and large, deal with communication channel capacity, stochastic analysis thereof, etc. These earlier systems treat information as a classical (non-quantum) entity. Modern day digital computers utilizing micron-sized transistors, although they are designed using quantum mechanical principles, are still dealing with large statistical ensembles of electrons to represent logical "1" and

"0" states. These large statistical ensembles are handled with statistical mechanics and measured with integrating volt/amp meters. So the present day information representation and processing technology, although faster than the wheels and gears of the Charles Babbage computation machine, is still in the same computational complexity class as the Babbage machine, with bits of information represented by entities which obey classical (non-quantum) physics. A significant amount of work in quantum computation deals with the impact of the quantum nature of the information upon practical device design.

Quantum information, as opposed to digital information of todays computers, is not representable without the laws of quantum physics. For example, a quantum state's information content originates from the following:

1. The state of a particle is represented by a vector $\mid \psi(t)\rangle$ in a Hilbert space: $\mathcal{H}$.

The above statement carries the implication that since $\mathcal{H}$ is a vector space, then there is a superposition principle for the vector $\mid \psi(t)\rangle$. That is, that a linear combination of vectors is a state vector:

$$\mid \psi(t)\rangle = \sum_{i=1}^{n} c_i \mid \omega(t)\rangle \tag{1.1}$$

This superposition property of q-bits implies that a binary quantum register (a register in which only the truth values up ($\uparrow$) and down($\downarrow$) - analogous to "1"and"0"of classical digital computer logic) has not only an admittable basis of 2^nstates, but also coherent superpositions of those 2^nstates. Eckert, gives the following simplified example of a three bit quantum register:[5]

$$\begin{aligned} \mid \Psi\rangle &= \sum_{x_2=\{0.1\}^3} c_{x_2} \mid x_2\rangle \\ &= c_{000} \mid\downarrow\downarrow\downarrow\rangle + c_{001} \mid\downarrow\downarrow\uparrow\rangle \\ +c_{010} &\mid \downarrow\uparrow\downarrow\rangle + c_{011} \mid\downarrow\uparrow\uparrow\rangle \\ +c_{100} &\mid \uparrow\downarrow\downarrow\rangle + c_{101} \mid\uparrow\downarrow\uparrow\rangle \\ +c_{110} &\mid \uparrow\uparrow\downarrow\rangle + c_{111} \mid\uparrow\uparrow\uparrow\rangle \end{aligned} \tag{1.2}$$

Where $x_2$indicates the binary (radix-2) number system and $\{0,1\}^3$indicates a three bit number. There are 2^ndifferent states of this register, which implies that 2^ndifferent numbers

could be represented. In the quantum superposed 2^n--dimensional Hilbert space, as opposed to the classical binary computer register, coherent superpositions of all of these states exist at once. This is quite different from classical computation. This fact gives remarkable power to the quantum computer over conventional digital computers: *A quantum computer can follow several paths at once.*

2. Any measurable state $\mid \Psi\rangle$ is described by an operator Ω acting in H and this operator is an observable. Thus a state is represented by an observable.

3. If a particle is in a sate $\mid \Psi\rangle$, then any measurement of the variable (corresponding to) Ω will give the eigenvalues ω with probability $P(\omega)$ $\alpha \mid \langle \omega \mid \Psi \rangle \mid^2$ .The result of measurement yields $\mid \omega\rangle$ from $\mid \Psi\rangle$.

4. The state vector obeys the Schrödinger equation (for the nonrelativistic case):

$$i\hbar \frac{d}{dt} \mid \Psi(t)\rangle = H \mid \Psi(t)\rangle \tag{1.3}$$

The relativistic case is treated by the Dirac Equation.[7]

Returning to the measurement problem, it appears that the measurement of the variable Ω changes the state, which is a superposition of the form:

$$\mid \Psi\rangle = \sum_{\omega} \mid \omega\rangle\langle\omega \mid \Psi\rangle \tag{1.4}$$

collapsing the state into the eigenstate $\mid \omega\rangle$.

The effect of the measurement of the state as discussed above, leads to a discussion of reversibility of measurements and hence to reversible computation. Current digital logic in conventional computers is irreversible. This leads to considerations of fan-out— the number of gates which may be driven from (or connected to) another gate. Irreversibility implies some minimum dissipation associated with computation. The unitary nature of quantum computations (and hence their reversible nature) departs significantly from the afore stated irreversible computational elements of present -day computation. Thus, the type of algorithms a quantum computer is capable of running force us to re-think the physics of the computation — that is, to derive a new theory of information representation commensurate with quantum systems. This hits at the very foundations of present state of the art of

computational science — so much so, that the quantum computation community speaks of "reprogramming the computer scientists to learn the physics of quantum information theory.

As discussed above, the unitarity hence reversibility of quantum transformations gives the quantum computer designer the ability to greatly increase algorithm parallelism through the ability to operate on not just a "quantum register" (q-register) but also on a coherent superposition of states of that q-register. In terms of computational complexity classes, this yields an exponential increase in computational speed for computationally hard problems like factoring. The problem of deriving quantum information theory is being viewed as a community-wide problem by this program through the work of Schulman and Privman at Clarkson University[6] .

Furthermore, the effects of decoherence upon a state is also of fundamental interest for quantum memory implementation. This is a consequence of the statement that there's no free lunch. Consider the standard quantum mechanical problem of a particle in a box. Each interaction with the box or any outside entity causes decoherence. Decoherence limits the power of quantum computation. However, the way that we obtain the result of calculations from the computer is through interactions. The problem of deriving theories and practical work-arounds to decoherence effects is being considered in this program.

To summarize, this program is in the earliest stages of derivation of fundamentals of quantum information theory as applied to quantum computational concepts. The eventual goal is to derive quantum mechanical computers in the solid state. The early experimental and theoretical work in this area by this author and others[8] is a starting point, but much work needs to be done to continue to a physical realization of an operational quantum computational engine.

Chapter 1 presents the application of the concept of quantum information to the derivation of the interaction Hamiltonians corresponding to the quantum NOT and EXCLUSIVE-OR (XOR) gates. The spin Hamiltonians synthesized in Chapter 1 are generalized and applied to a system containing both electronic and nuclear spins in an Electron-Nuclear Double Resonance (ENDOR) formulation of quantum gate structures in Chapter 2. The derivation of a radix R>2 quantum computational scheme is presented in Chapter 3. A summary is presented in Chapter 4.

Chapter 1

Design of Gates for Quantum Computation

As discussed in the preface, the problem of logic design for quantum computation is very different than that for present-day digital computers. In this chapter, the result of considering quantum spin systems to be the physical realization of quantum bits (q-bits) is carried to the design of quantum logic gates. As expected, the first step in the design of quantum logic gates is the derivation of the interaction Hamiltonian corresponding to the gate operation. This is followed by an analysis of its properties and realization in a physical system. At present, the first two steps have been performed by our group (Hotaling at Rome Lab, and Privman et.al. at Clarkson University), while the last step, the critical quantum engineering has yet to be performed. The earlier experiments by the author and others, have operated upon statistical ensembles of spin systems, but singlet states must be used to fully utilize the computational complexity (read power) of quantum computation; Sustainable coherent states must be generated, manipulated and interfaced to the macroscopic world. The first section presents the quantum NOT gate design. The next sections discuss the quantum exclusive or (XOR) gate in terms of two- and three-spin interactions, respectively.

1.1 The Quantum NOT Gate Hamiltonian

This section was published as a paper in the International Journal of Modern Physics B in 1997, and hence, the present section is a preprint of that paper.

DESIGN OF GATES FOR QUANTUM COMPUTATION: THE NOT GATE

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We offer an alternative to the conventional network formulation of quantum computing. We advance the *analog* approach to quantum logic gate/circuit construction. As an illustration, we consider the *spatially extended* NOT gate as the first step in the development of this approach. We derive an explicit form of the interaction Hamiltonian corresponding to this gate and analyze its properties. We also discuss general extensions to the case of certain time-dependent interactions which may be useful for practical realization of quantum logic gates.

1. Introduction

The fundamental physics of reversible quantum-mechanical computation has received much attention recently.[1] Quantum computer is a hypothetical quantum-coherent system that functions as a programmable calculational apparatus. Such a computer will have to be drastically different from its classical counterparts. It will enable solution of certain problems[1] much faster than the classical computer: the quantum interference property yields[1] the fast-factoring (Shor's), as well as certain other fast algorithms. Recent theoretical results have included identification of universal reversible two-bit gates[2] and advances[3] in error correction. There have also been experiments[4] realizing a simple gate.

Nevertheless, the idea of construction of a macroscopic computer out of a large number of quantum bits (qubits) is ellusive[5] at the present stage of technology. The main obstacle is the sensitivity of coherent quantum evolution and interference to undesirable external interactions such as noise or other failures in operation.[1,5,6] Even though a number of error correction schemes have been proposed,[3] not all types of error can be corrected. This particularly applies to the *analog* nature of quantum computers[6] which will be addressed below.

Quantum computers are naturally analog in their operation because in order to use the power of quantum interference, one has to allow any linear combination of

the basis qubit states. By analog errors we mean those minor variations in the input and output variables and in the system's dynamics which cannot on their own be identified as erroneous in an analog device because its operation involves continuous values of variables (so that the fluctuated values are as legal as the original ones). By noise errors we mean those that result from single-event problems with device operation, or from external influences, or from other failures in operation. In the quantum case the latter errors also include the decoherence effects due to influences of the environment.

Error-correction techniques can handle the noise errors but not the analog errors. Indeed consider a state $\alpha|1\rangle + \beta|0\rangle$ and a nearby state $\alpha'|1\rangle + \beta'|0\rangle$, where α' is close to α, while β' is close to β. Here $|1\rangle$ and $|0\rangle$ denote the basis qubit or spin states in the notation reminiscent of the classical bit states 1 and 0. Both linear-superposition states are equally legal as input or output quantum states. Furthermore in the conventional picture of a quantum computer[1] which assumes a network of a multitude of simple gate-units each being controlled externally, the analog errors can proliferate and be magnified in each step of the computation.

In this work we therefore adopt a view typical of the "classical" analog computer approach, of designing the computer as a *single unit* performing in one-shot a complex logical task instead of a network of simple gates each performing a simple "universal-set" logical function. In this case the computer as a whole will still be subject to analog errors. However, these will not be magnified by proliferation of sub-steps each of which must be exactly controlled. Indeed, quantum (and more generally reversible) computation must be externally timed: the time scale of the operation of each gate is determined by the interactions rather than by the relaxation processes as in the ordinary computer. Furthermore, gate interactions must be externally switched[1] on and off because the gates affect each other's operation.

In fact, we consider it likely that technological advances might first allow design and manufacturing of limited size units, based on several tens of atomic two-level systems, operating in a coherent fashion over sufficiently large time interval to function as parts of a larger classical (dissipative) computer which will not maintain quantum coherent operation over its macroscopic dimensions. We would like these to function as single analog units rather than being composed of many gates.

While in principle in a reversible computational unit input and output spins (qubits) need not be different, for larger units interacting with the external world it may be practically useful to consider input and output separate (or at least not identical). Indeed, the interactions that feed in the input need not necessarily be identical to those interactions/measurements that read off the output.

In light of these considerations we consider in this work a *spatially extended* NOT gate based on two spins: one input and one output. Actually, we have to address a complicated set of problems: can multispin computational units be designed with short-range, two-particle interactions? Can they accomplish logical functions with interactions of the form familiar in condensed matter or other experimental systems? These and similar questions can only be answered by multispin-unit calculations

which will have to be numerical. Analytical results are limited to the simplest gates such as NOT and XOR, the latter studied in Ref. 7, and they provide only a partial picture.

This work is organized as follows. In Sec. 2 we consider a simple, "textbook" example: the one-qubit NOT gate. It is considered for illustration only and allows us to introduce the notation in a simple setting and exemplify some general ideas. In Sec. 3 we consider the NOT gate with spatially separated input and output qubits. The interaction Hamiltonian derived for this gate, Eq. (21) below, establishes that it can be operated by the internal interactions alone so that external-field effects can perhaps be reserved for the clocking of the internal interactions. Furthermore, it suggests the type of local internal interactions to be used in more complicated systems where the computer as a whole is treated as a many-body system with time-independent interactions.

The conventional formulation[1] of quantum computing involves the external on and off switching of the interactions. In Sec. 4, we show that this requirement can be relaxed and the time dependence be given by other time-dependent interactions (protocols) which are smoother than the on/off shape. Section 4 also offers a summarizing discussion.

2. The Simple NOT Gate

In this section we consider the NOT gate based on a two-state system. Such a gate has been extensively studied in the literature,[1] so that our discussion is a review intended to set up the notation and illustrate methods useful in more complicated situations. We label by $\binom{1}{0}$ and $\binom{0}{1}$ the two basis states. The NOT gate corresponds to those interactions which, over the time interval Δt, accomplish the following changes:

$$\binom{1}{0} \Longrightarrow e^{i\alpha}\binom{0}{1}, \tag{1}$$

$$\binom{0}{1} \Longrightarrow e^{i\beta}\binom{1}{0}. \tag{2}$$

The phases α and β are arbitrary. The unitary matrix U, that corresponds to this evolution, is uniquely determined,

$$U = \begin{pmatrix} 0 & e^{i\beta} \\ e^{i\alpha} & 0 \end{pmatrix}. \tag{3}$$

The eigenvalues of U are given by

$$u_1 = e^{i(\alpha+\beta)/2} \quad \text{and} \quad u_2 = -e^{i(\alpha+\beta)/2}, \tag{4}$$

while the eigenvectors, when normalized and regarded as matrix columns, yield the following transformation matrix T which can be used to diagonalize U:

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} \\ e^{i\alpha/2} & -e^{i\alpha/2} \end{pmatrix} . \tag{5}$$

Thus, we have

$$T^\dagger U T = \begin{pmatrix} u_1 & 0 \\ 0 & u_2 \end{pmatrix} . \tag{6}$$

Here the dagger superscript denotes Hermitian conjugation.

We next use the general relation

$$U = e^{-iH\Delta t/\hbar} \tag{7}$$

to identify the time-independent Hamiltonian in the diagonal representation. Relations (4) yield the energy levels:

$$\begin{aligned} E_1 &= -\frac{\hbar}{2\Delta t}(\alpha+\beta) + \frac{2\pi\hbar}{\Delta t} N_1 , \\ E_2 &= -\frac{\hbar}{2\Delta t}(\alpha+\beta) + \frac{2\pi\hbar}{\Delta t}\left(N_2 + \frac{1}{2}\right) , \end{aligned} \tag{8}$$

where N_1 and N_2 are arbitrary integers. The Hamiltonian is then obtained from the relation

$$H = T \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} T^\dagger \tag{9}$$

as a certain 2×2 matrix. The latter is conveniently represented in terms of the unit matrix $\mathcal{I}$ and the conventional Pauli matrices σ_x, σ_y, σ_z. We get

$$\begin{aligned} H = &\left[-\frac{\hbar}{2\Delta t}(\alpha+\beta) + \frac{\pi\hbar}{\Delta t}\left(N_1 + N_2 + \frac{1}{2}\right)\right]\mathcal{I} \\ &+ \frac{\pi\hbar}{\Delta t}\left(N_1 - N_2 - \frac{1}{2}\right)\left[\left(\cos\frac{\alpha-\beta}{2}\right)\sigma_x + \left(\sin\frac{\alpha-\beta}{2}\right)\sigma_y\right] . \end{aligned} \tag{10}$$

To effect the gate operation, the interaction must be switched on for the time interval Δt. The constant part of the interaction energy (the part proportional to the unit matrix $\mathcal{I}$) is essentially arbitrary; it only affects the average phase $(\alpha+\beta)/2$ of the transformation (1)–(2). Thus this term can be omitted.

The nontrivial part of (10) depends on the integer $N = N_1 - N_2$ which is arbitrary, and on one arbitrary angular variable

$$\gamma = \frac{\alpha-\beta}{2} . \tag{11}$$

Thus we can use the Hamiltonian in the form

$$H = \frac{\pi\hbar}{\Delta t}\left(N - \frac{1}{2}\right)[(\cos\gamma)\sigma_x + (\sin\gamma)\sigma_y] . \tag{12}$$

For a spin-1/2 two-state system such an interaction can be obtained by applying a magnetic field oriented in the XY-plane at an angle γ with the X-axis. The strength of the field is inversely proportional to the desired time interval Δt, and various allowed field values are determined by the choice of N.

We note that during application of the external field the *up* and *down* quantum states in (1)–(2) are *not* the eigenstates of the Hamiltonian. If the time interval Δt is not short enough, the energy-level splitting $|E_1 - E_2| \propto |N - \frac{1}{2}|$ can result in spontaneous emission which is just one of the undesirable effects destroying quantum coherence. Generally, when implemented in a condensed matter matrix for instance, the two states of the qubit may lie within a spectrum of various other energy levels. In that case, in order to minimize the number of spontaneous transition modes, the best choice of the interaction strength would correspond to minimizing $|E_1 - E_2|$, i.e., to $|N - \frac{1}{2}| = \frac{1}{2}$.

3. The Spatially Extended NOT Gate

In this section we consider a spatially extended NOT gate consisting of two spins: input and output. We will describe these spins by four-state vectors and matrices labeled according to the following self-explanatory convention:

$$\begin{aligned}\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} &= a_1|\uparrow\uparrow\rangle + a_2|\uparrow\downarrow\rangle + a_3|\downarrow\uparrow\rangle + a_4|\downarrow\downarrow\rangle \\ &= a_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\mathrm{I}} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\mathrm{O}} + a_2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\mathrm{I}} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\mathrm{O}} \\ &\quad + a_3 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\mathrm{I}} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}_{\mathrm{O}} + a_4 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\mathrm{I}} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix}_{\mathrm{O}} . \end{aligned} \tag{13}$$

Here I and O denote *Input* and *Output*. In what follows we will omit the direct-product symbols $\otimes$ when multiplying expressions with subscripts I and O.

The desired transformation should take any state with $a_3 = a_4 = 0$ into a state with components 1 and 3 equal zero, i.e., *Input up* yields *Output down*. Similarly, any state with $a_1 = a_2 = 0$ should evolve into a state with components 2 and 4 equal zero, corresponding to *Input down* giving *Output up*. The general evolution operator must therefore be of the form

$$U = \begin{pmatrix} 0 & 0 & U_{13} & U_{14} \\ U_{21} & U_{22} & 0 & 0 \\ 0 & 0 & U_{33} & U_{34} \\ U_{41} & U_{42} & 0 & 0 \end{pmatrix}, \tag{14}$$

which depends on 16 real parameters. However, one can show that the requirement of unitarity, $U^\dagger U = 1$, imposes 8 conditions so that the number of real parameters is reduced to 8. A lengthy but straightforward algebraic calculation then shows

that the following parametrization covers all such unitary matrices:

$$U = \begin{pmatrix} 0 & 0 & e^{i\chi}\sin\Omega & e^{i\beta}\cos\Omega \\ -e^{i(\alpha+\rho-\eta)}\sin\Upsilon & e^{i\rho}\cos\Upsilon & 0 & 0 \\ 0 & 0 & e^{i\delta}\cos\Omega & -e^{i(\beta+\delta-\chi)}\sin\Omega \\ e^{i\alpha}\cos\Upsilon & e^{i\eta}\sin\Upsilon & 0 & 0 \end{pmatrix} . \tag{15}$$

Here all the angular variables are unrestricted although we could limit Ω and Υ to the range $[0, \pi/2]$ without loss of generality.

In order to make the calculation analytically tractable, we will restrict the number of free parameters to four by considering the case

$$U = \begin{pmatrix} 0 & 0 & 0 & e^{i\beta} \\ 0 & e^{i\rho} & 0 & 0 \\ 0 & 0 & e^{i\delta} & 0 \\ e^{i\alpha} & 0 & 0 & 0 \end{pmatrix} . \tag{16}$$

This form has been favored for the following reasons. Firstly, the structure of a single phase-factor in each column is similar to that of the two-dimensional matrix encountered in Sec. 2. Secondly, the form (16) contains Hermitian-U cases ($\beta = -\alpha$, $\rho = 0$ or π, $\delta = 0$ or π). Therefore, the eigenvalues, which are generally on the unit circle for any unitary matrix, may be positioned more symmetrically with respect to the real axis. as functions of the parameters. These observations suggest that an analytical calculation may be possible.

Indeed, the eigenvalues of U turn out to be quite simple:

$$u_1 = e^{i(\alpha+\beta)/2}, \quad u_2 = -e^{i(\alpha+\beta)/2}, \quad u_3 = e^{i\rho}, \quad u_4 = e^{i\delta} . \tag{17}$$

The diagonalizing matrix T made up of the normalized eigenvectors as columns is

$$T = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\beta/2} & e^{i\beta/2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{2} \\ e^{i\alpha/2} & -e^{i\alpha/2} & 0 & 0 \end{pmatrix} . \tag{18}$$

The next step in the calculation is to identify the energy levels. We chose the notation such that the energies $E_{1,2}$ are identical to (8). The other two energies are given by

$$E_3 = -\frac{\hbar}{\Delta t}\rho + \frac{2\pi\hbar}{\Delta t}N_3 , \quad E_4 = -\frac{\hbar}{\Delta t}\delta + \frac{2\pi\hbar}{\Delta t}N_4 , \tag{19}$$

The Hamiltonian is then obtained as in Sec. 2. It is convenient to avoid cumbersome expressions by expressing it in terms of the energies; the latter will be replaced by explicit expressions (8), (19) when needed. The resulting 4×4 matrix has been expressed in terms of the direct products involving the unit matrices and

the Pauli matrices of the *Input* and *Output* two-state systems. This calculation is straightforward but rather lengthy. We only report the result:

$$H = \frac{1}{4}(2E_1 + 2E_2 + E_3 + E_4) + \frac{1}{4}(E_3 - E_4)(\sigma_{z\mathrm{I}} - \sigma_{z\mathrm{O}})$$
$$+ \frac{1}{4}(2E_1 + 2E_2 - E_3 - E_4)\sigma_{z\mathrm{I}}\sigma_{z\mathrm{O}}$$
$$+ \frac{1}{4}(E_1 - E_2)\left(\cos\frac{\alpha-\beta}{2}\right)(\sigma_{x\mathrm{I}}\sigma_{x\mathrm{O}} - \sigma_{y\mathrm{I}}\sigma_{y\mathrm{O}})$$
$$+ \frac{1}{4}(E_1 - E_2)\left(\sin\frac{\alpha-\beta}{2}\right)(\sigma_{x\mathrm{I}}\sigma_{y\mathrm{O}} + \sigma_{y\mathrm{I}}\sigma_{x\mathrm{O}}). \qquad (20)$$

As in Sec. 2, we note that the constant part of the Hamiltonian can be changed independently of the other coupling constants and it can be discarded. Recall that we can generally vary the integers $N_{1,2,3,4}$ and the variables α, β, ρ, δ. The "constant" part is in fact proportional to $\mathcal{I}_\mathrm{I} \otimes \mathcal{I}_\mathrm{O}$. However, we avoid this cumbersome notation and present the terms in the Hamiltonian in a more physically transparent form.

The Hamiltonian in (20) has also terms linear in the Pauli matrices (in the spin components for spin systems). These correspond to interactions with externally applied fields which in fact must be of opposite direction for the *Input* and *Output* spins. We try to avoid such interactions: hopefully, external fields will only be used for "clocking" of the computation, i.e., for controlling the internal interactions of the *Input* and *Output* two-state systems. Thus, we will assume that $E_3 = E_4$ so that there are no terms linear in the spin components, in the Hamiltonian.

Among the remaining interaction terms, the term involving the z-components in the product form $\sigma_{z\mathrm{I}}\sigma_{z\mathrm{O}}$ ($\equiv \sigma_{z\mathrm{I}} \otimes \sigma_{z\mathrm{O}}$), has an arbitrary coefficient, say, $\mathcal{E}$. The terms of order two in the x and y components have free parameters similar to those in (11)–(12) in Sec. 2. The final expression is

$$H = -\mathcal{E}\sigma_{z\mathrm{I}}\sigma_{z\mathrm{O}}$$
$$+ \frac{\pi\hbar}{2\Delta t}\left(N - \frac{1}{2}\right)\left[(\cos\gamma)\,(\sigma_{x\mathrm{I}}\sigma_{x\mathrm{O}} - \sigma_{y\mathrm{I}}\sigma_{y\mathrm{O}}) + (\sin\gamma)\,(\sigma_{x\mathrm{I}}\sigma_{y\mathrm{O}} + \sigma_{y\mathrm{I}}\sigma_{x\mathrm{O}})\right]. \qquad (21)$$

Here $N = N_1 - N_2$ must be integer. In order to minimize the spread of the energies E_1 and E_2 we could choose $|N - 1/2| = 1/2$ as in Sec. 2. Recall that we already have $E_3 = E_4$. Actually, the energy levels of the Hamiltonian in the notation (21) are

$$E_1 = -\mathcal{E} + \frac{\pi\hbar}{\Delta t}\left(N - \frac{1}{2}\right), \quad E_2 = -\mathcal{E} - \frac{\pi\hbar}{\Delta t}\left(N - \frac{1}{2}\right), \quad E_{3,4} = \mathcal{E}. \qquad (22)$$

Thus further degeneracy (of three levels but not all four) can be achieved by varying the parameters.

4. Time-Dependent Interactions. Discussion

The form of the interactions in (21) is quite unusual as compared to the traditional spin-spin interactions in condensed matter models. The latter usually are based on the uniaxial (Ising) interaction proportional to $\sigma_z\sigma_z$, or the planar XY-model interaction proportional to $\sigma_x\sigma_x+\sigma_y\sigma_y$, or the isotropic (scalar-product) Heisenberg interaction. The spin components here are those of two different spins (not marked). The interaction (21) involves an unusually high degree of anisotropy in the system. The x and y components are coupled in a tensor form which presumably will have to be realized in a medium with well-defined directionality, possibly, a crystal.

All the interaction Hamiltonians considered thus far were constant for the duration of the gate operation. They must be externally controlled. However, we note that the application of the interaction need not be limited to the time-dependence which is an abrupt on/off switching. Indeed, we can modify the time dependence according to

$$H(t) = f(t)H\,, \tag{23}$$

where we use the same symbol H for both the original time-independent interaction Hamiltonian such as (21) and the new, time-dependent one, $H(t)$. The latter involves the "protocol" function $f(t)$. The shape of this function, nonzero during the operation of the gate from time t to time $t+\Delta t$, can be smooth.

For Hamiltonians involving externally applied fields, such as (12), it may be important to have a constant plus an oscillatory components (corresponding to constant and electromagnetic-wave magnetic fields, for instance). However, the protocol function must satisfy

$$\int_t^{t+\Delta t} f(t')\,dt' = \Delta t\,, \tag{24}$$

and therefore it cannot be purely oscillatory; it must have a constant or other contribution to integrate to a nonzero value in accordance with (24).

The possibility of the modification (23) follows from the fact that the general relation

$$U = \left[e^{-i\int_t^{t+\Delta t} H(t')\,dt'/\hbar}\right]_{\text{time-ordered}} \tag{25}$$

does not actually require time ordering as long as the Hamiltonian commutes with itself at different times. This condition is satisfied by (23). Furthermore, if the Hamiltonian can be written as a sum of commuting terms then each term can be multiplied by its own protocol function. Interestingly, the Hamiltonian of the "paramagnetic resonance" NOT gate, reviewed by DiVincenzo in Refs. 1, is not of this form. It contains a constant part and an oscillatory part but they do not commute. Note that the term proportional to $\mathcal{E}$ in (21) commutes with the rest of that Hamiltonian. The terms proportional to $\cos\gamma$ and $\sin\gamma$ do not commute with each other though. Rather, they anticommute, in (21), as such terms do in (12).

In summary, we have derived expressions for the interaction Hamiltonians appropriate for the NOT gate operation in two-state systems. The expressions obtained will be useful in identifying materials where there is hope of actually realizing such gates, in writing down model Hamiltonians for more complicated, multispin configurations, and in studying these gates as individual components, for instance, with dissipation added.

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1.2 The Two-Spin Exclusive-OR (XOR) Gate Hamiltonian

This section was published as a paper on the World Wide Web with the Los Alamos National Laboratory Quantum Physics web site. Hence, the present section is a preprint of that paper.

Extended Quantum XOR Gate in Terms of Two-Spin Interactions

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ABSTRACT

The analog nature of quantum computing makes constructing logical operations from many simple gates inappropriate. We explain this and then propose to design multispin quantum gates in which the input and output two-state systems (spins) are not necessarily identical. We outline the design criteria for such devices and consider an example of a two-spin interaction Hamiltonian which accomplishes the quantum XOR gate function for a system of three spins: two input and one output.

Dimensions of semiconductor computer components will soon reach [1] about $0.25\,\mu\mathrm{m} = 2500\,\text{Å}$, which is well above the atomic sizes. However, it is generally expected that in time atomic dimensions will be reached and coherent quantum computing will have to be explored. Some studies [2] have considered how quantum mechanics affects the foundations of computer science, e.g., limitations on classical computation due to quantum fluctuations, etc. A more recent development [3] has been to utilize the quantum-coherent nature of components of atomic dimensions for more efficient computations.

Quantum computing may be faster than classical computing [3]. Error correction techniques [4], unitary operations corresponding to the simplest logic gates [3] and some Hamiltonians for gate operation have been explored. Ideas on how to combine the simplest quantum gates have been put forth [5]. Experimentally, there are several atomic-scale systems where the simplest quantum-gate functions have been recently realized [6] or contemplated [3,7].

There remain, however, many conceptual difficulties with quantum computing [2,3]. The reversibility of coherent quantum evolution implies that the time scale Δt of the operation of quantum logic gates must be built into the Hamiltonian. As a result, all the proposals available to date assume that computation will be externally timed, i.e., interactions will

be switched *on* and *off*, for instance, by laser radiation.

This implies that if logical operations are constructed from a small set of simple gates, then each such gate will have to be precisely controlled from outside. In ordinary classical (i.e., macroscopic, irreversible) computing, the NAND gate is an example of a universal gate. From it complicated logical operations can be constructed. In the classical case, however, it is the internal relaxation processes in the basic-set gate(s) that determine the time scale of their operation (equilibration) Δt. We consider it extremely unlikely that one would ever be able to control externally, in a coordinated fashion, millions of simple reversible quantum gates in order to operate a macroscopic computer.

Furthermore, quantum computers are naturally *analog* [8] in their operation. In order to use the power of quantum superposition of states, one has to allow linear combinations of the basis qubit states $|1\rangle$ and $|0\rangle$. Analog errors are difficult to correct. By analog errors we mean those minor variations in the input and output variables which cannot on their own be identified as erroneous in an analog device because its operation involves *continuous* values of variables (so that the fluctuated values are as legal as the original ones). By noise errors we term those that result from single-event problems with device operation, or from external influences that include decoherence in the quantum case, or from other

failures in operation. All errors in a *digital* device (i.e., deviations from correct discrete values) can be systematically decreased or eliminated in each step of a calculation. Similarly, the noise errors in analog devices can be corrected or decreased.

However, the analog errors cannot be corrected. Consider a state $\alpha|1\rangle + \beta|0\rangle$ and a nearby state $\alpha'|1\rangle + \beta'|0\rangle + \sum_j \zeta_j|j\rangle$, where α' is close to α, β' is close to β, while ζ_j are small. The latter terms represent possible admixture of quantum states $|j\rangle$ other than the two qubit states. Indeed, it is likely that a multistate atomic-dimension system will be used with two particular states serving as the two-state "qubit." Both states are equally legal as input and output quantum states. We could restrict input or output to a vicinity of certain states, for instance, the basis states $|1\rangle$ and $|0\rangle$, thus moving towards digitalization. However, we then loose the quantum-interference property. Another important effect, decoherence, that would require a density matrix description, falls in the noise-error category.

Modern error-correction techniques [3,4] can handle the noise errors but not the analog errors. Thus they mainly focus on decoherence effects due to environment in a particular quantum state and on how to minimize these affects in storing the state and transmitting it. The analog errors in *computation* as a dynamical process, though, cannot be corrected this

way. To illustrate, consider this quote [9] from the article entitled *Quantum Error Correction for Communication*: "To achieve this the sender can add two qubits, initially both in state $|0\rangle$, to the original qubit and then perform an encoding unitary transformation...". The problem here is that the states actually encountered in the system during error correction are not available as basis qubit states (such as $|0\rangle$) with infinite precision.

Typically, by qubits we mean a set of two orthogonal quantum states selected from the energy eigenstates of an ideal atomic system. Even assuming that the thermal noise can be reduced at low temperatures to make the ground state sufficiently long-lived, the excited states of any system, especially if it is a part of a macroscopic computer, will not be defined sharply enough to provide ideal stationary states $|1\rangle$ and $|0\rangle$. External interactions, spontaneous emissions, etc., will generate both noise- and analog-errors in the basis states (as well as in their superposition that is our wavefunction), i.e., the actual state (disregarding decoherence) will be $\alpha|1\rangle + \beta|0\rangle + \sum_j \zeta_j|j\rangle$, with $\alpha \simeq 1$ and $\beta, \zeta_j \simeq 0$, instead of $|1\rangle$ which is an eigenstate of an ideal, isolated-system Hamiltonian, etc.

Furthermore, analog errors will be magnified when separate simple-gate operations are combined to yield a complex logical function. Thus, the conventional picture [3] of a quantum computer is unrealistic: it

assumes a multitude of simple-gate units each being externally controlled by laser beams in an exactly coordinated manner. Such computers will magnify analog errors which cannot be corrected in principle because the error state is as legal as the original state.

In this work we therefore adopt a view typical of the "classical" analog-computer approach, of designing the computer as a single unit performing in one shot a complex logical task instead of a chain of simple gate tasks. This approach will not repair all the ailments outlined earlier. For instance, the computer as a whole will still be subject to analog errors. However, these will not be magnified by proliferation of sub-steps each of which must be exactly controlled.

In fact, we consider it likely that technological advances might first allow design and manufacturing of limited-size units, based on several tens of atomic two-level systems, operating in a quantum-coherent fashion over a sufficiently large time span to function as parts of a larger classical (dissipative) computer which will not maintain a quantum-coherent operation over its macroscopic dimensions. We would like these to function as single analog units rather then being composed of many gates. In the rest of this work, we first offer some design considerations for such multispin quantum units and then present a simple illustrative example of a three-spin unit that performs the quantum XOR function.

In order to make connections with the classical computer-circuitry design and identify, at least initially, which multi-qubit systems are of interest, we propose to consider spatially extended multispin quantum gates with input and output qubits possibly different. The reason for emphasizing this property is that multispin devices will have spatial extent. The interactions that feed the input need not be identical to those interactions/measurements that read off the output. Furthermore, for systems with short-range interactions one can only access the boundary spins in a large cluster. Thus we may use only part of the spins to specify the input and another subset to contain the output. The two sets may be identical, partially overlapping, or nonoverlapping. Reversibility of coherent quantum evolution makes the distinction between the input and output less important than in irreversible computer components. However, we consider the notion of separate (or at least not necessarily fully identical) input and output useful within our general goals: to learn what kind of interactions are involved and to consider also units that might be connected to/as in classical (dissipative) computer devices.

Our goal is to be able to design interaction parameters, presumably by numerical simulations, to have such gates perform useful Boolean operations. This is not an easy task. Actually, it must be broken into several steps. First, we must identify those interactions which can be realized in solid state or other experimental arrangements. As the XOR

example below illustrates [10], the form of the interaction Hamiltonians may be quite unusual by the solid-state standards. Secondly, we expect interactions to be short-range and two-particle (two-spin) when several two-state systems (termed here qubits or spins) are involved.

Thirdly, incorporating designed coherent computational units in a larger classical computer will require a whole new branch of computer engineering because the built-in Boolean functions will be complicated as compared to the conventional NOT, AND, OR, NAND, etc., to which computer designers are accustomed. Furthermore, the rules of their interconnection with each other and with the rest of the classical computer will be different from today's devices.

Our initial studies have been analytical [10]. In the future we foresee numerical studies of systems of order 20 to 25 two-state (spin) atomic components with variable general-parameter interactions. Consideration of multispin quantum gates requires a large number of basis states. However, it is also useful to study few-spin exactly solvable systems [10]. These provide explicit examples of what the actual interaction Hamiltonians should look like.

An accepted approach has been to consider interactions switched on only for the duration of the gate operation Δt. If the gate is actually the whole computer then one can regard the interaction as time-independent.

However, for specific tasks in components with a limited number of basis states, it may be appropriate to view the interaction as controlled externally to be switched on and off. While general ideas of externally timed computation are not new [2], actual realizations in quantum computation with many sub-unit gates will encounter difficulties outlined earlier.

With regards to the requirement to control the interactions externally, with the time dependence given by the on/off protocol, we have shown [10] that a smoother time-dependence is possible, with the original Hamiltonian H, which is constant over the time interval Δt, replaced by $f(t)H$, where the protocol function $f(t)$ averages to 1 over the time interval Δt.

Let us now turn to the XOR-gate example. We will use the term "spin" to describe a two-state system, and we will represent spin-$\frac{1}{2}$-particle spin-components (measured in units of $\hbar/2$) by the standard Pauli matrices $\sigma_{x,y,z}$. In Figure 1, we denote by A, B, C the three two-state systems, i.e., three spins, involved. We assume that at time t the input spins A and B are in one of the basis states $|AB\rangle = |11\rangle$, $|10\rangle$, $|01\rangle$, or $|00\rangle$, where 1 and 0 denote the eigenstates of the z-component of the spin operator, with 1 referring to the "up" state and 0 referring to the "down" state. We use this notation for consistency with the classical "bit" notion. The initial state of C is not specified (it is arbitrary).

We would like to have a quantum evolution which, provided A and B are initially in those basis states, mimics the truth table of XOR:

A	B	output
1	1	0
1	0	1
0	1	1
0	0	0

(1)

were the output is at time $t + \Delta t$. One way to accomplish this is to produce the output in A or B, i.e., work with a two-spin system where the input and output are the same. The Hamiltonian for such a system is not unique. Explicit examples are known [3,5,11] where XOR was obtained as a sub-result of the controlled-NOT gate operation. In this case of two spins involved, the interactions can be single- and two-spin only.

However, here we want a multispin example, with emphasis on whether one can design interactions to be two-spin only and still accomplish "in one shot" the desired logical function. Thus, we require that the XOR result will be generated in C at time $t + \Delta t$. The final states of A and B, as well as the phase of C are arbitrary. In fact, there are many different unitary transformations, U, that correspond to the desired evolution in the eight-state space with the basis $|ABC\rangle = |111\rangle$, $|110\rangle$, $|101\rangle$, $|100\rangle$, $|011\rangle$, $|010\rangle$, $|001\rangle$, $|000\rangle$, which we will use in this order. The choice of the transformation determines what happens when the initial state is a

superposition of the reference states, what are the phases in the output, etc. The transformation is definitely not unique.

Consider the following Hamiltonian [10],

$$H = \frac{\pi\hbar}{4\Delta t}\left(\sqrt{2}\sigma_{zA}\sigma_{yB} + \sqrt{2}\sigma_{zB}\sigma_{yC} - \sigma_{yB}\sigma_{xC}\right) \tag{2}$$

It is written here in terms of the spin components. In the eight-state basis specified earlier, its matrix can be obtained by direct product of the Pauli matrices and unit 2×2 matrices $\mathcal{I}$. Here the subscripts A, B, C denote the spins. For instance, the first interaction term is proportional to $\sigma_{zA} \otimes \sigma_{yB} \otimes \mathcal{I}_C$, etc.

This Hamiltonian involves only two-spin-component interactions. In fact, A and C only interact with B, see Figure 1, so diagrammatically there is no loop (it is not known if the latter property is significant since we are dealing here with "nonequilibrium," i.e., non-ground-state, calculations).

One can show [10] that the Hamiltonian (2) corresponds to the XOR result in C at $t + \Delta t$ provided A and B where in one of the allowed superpositions of the appropriate "binary" states at t (we refer to superposition here because C is arbitrary at t). The actual "design" of the three-spin XOR gate with only two-spin interactions is quite complicated

[10].

The unitary matrix U that corresponds to the evolution over the time interval Δt, given by

$$U = \exp\left(-iH\Delta t/\hbar\right) = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \end{pmatrix} \tag{3}$$

and it corresponds to XOR in that any liner combination of the states $|\underline{1}\underline{1}1\rangle$ and $|\underline{1}\underline{1}0\rangle$ evolves into a linear combination of $|11\underline{0}\rangle$, $|10\underline{0}\rangle$, $|01\underline{0}\rangle$, and $|00\underline{0}\rangle$, compare the underlined quantum numbers with the first entry in (1), with similar rules for the other three entries in (1). It is straightforward to check that, with phase factors -1 in some cases, the unitary matrix U indeed places the XOR(A, B) in C. Note that (2) is not symmetric in A and B, so that another Hamiltonian can be obtained by relabeling.

We comment that both the XOR Hamiltonian (2) and other XOR and NOT gate Hamiltonians [10] studied in the present framework, are quite unusual as far as solid-state interactions go. They involve products of spin components. However, there is no obvious symmetry such as

uniaxial (Ising), planar (XY), isotropic (Heisenberg), familiar from the usual magnetic interactions in the solid state. Thus, while our example demonstrates that two-spin interaction Hamiltonians can be useful in generating standard logical operations in systems with more than two spins [10], general analytical results and more conventional solid-state interactions are difficult to come by in the framework of exactly solvable few-spin systems. It is likely that future quantum logic gate "design" will involve heavy numerical simulations of systems of several spins with trial, more conventional two-spin interactions, to determine interaction parameter values for which they perform useful logical operations.

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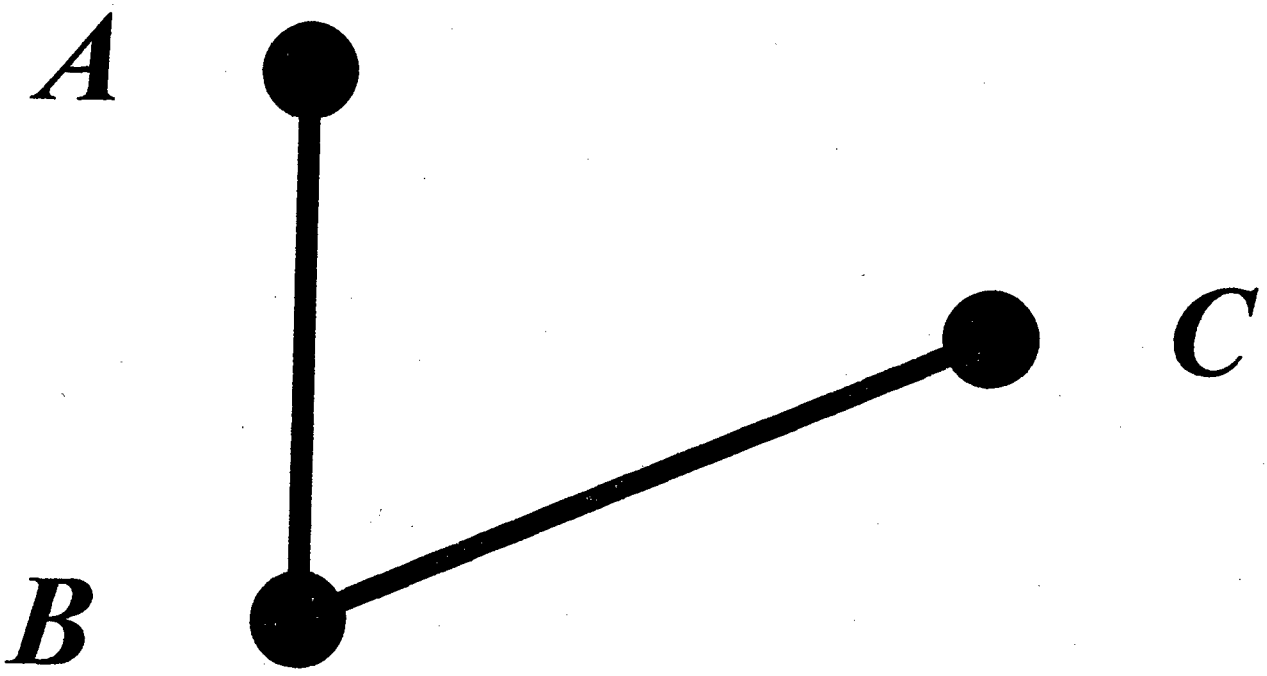

Figure 1: Three two-state systems (spins) A, B, C, with the pairwise spin-component interactions in (2) marked schematically by the connecting lines. The XOR operation accomplished by (2) in time Δt assumes that A and B are the input qubits and C is the output qubit.

1.3 The Three-Spin Exclusive -OR (XOR) Gate Hamiltonian

This section was published as a paper in the International Journal of Modern Physics B in 1997, and hence, the present section is a preprint of that paper.

Design of gates for quantum computation: the three-spin XOR in terms of two-spin interactions

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ABSTRACT

We propose to design multispin quantum gates in which the input and output two-state systems (spins) are not necessarily identical. We describe the motivations for such studies and then derive an explicit general *two-spin interaction* Hamiltonian which accomplishes the quantum XOR gate function for a system of three spins: two input and one output.

1. Introduction

Dimensions of semiconductor computer components will soon reach [1] about $0.25\,\mu\text{m} = 2500\,\text{Å}$, still well above the sizes at which quantum-mechanical effects are important. However, it is generally expected that as the miniaturization continues, atomic dimensions will be reached, perhaps, with technology different from today's semiconductors. Lead by this expectation, some early studies [2-4] considered how quantum mechanics affects the foundations of computer science; issues such as limitations on "classical" computation due to quantum fluctuations, etc., have been raised.

A more recent approach [4-30] has been to utilize the quantum nature of components of atomic dimensions for more efficient computation and design; this involves many interesting scientific concepts new to both computer science and physics. Several issues must be addressed. Is quantum computation faster than classical computation? Can quantum computational elements be built and combined with other quantum and/or classical components? What will be the "design" rules for quantum computer components in order to perform Boolean logic operations on quantum bits (qubits) such as the up and down spin states of a spin-$\frac{1}{2}$ particle? What are the error correction requirements and methods in

quantum computation?

Answers to most of these questions are still not known. However, some definitive results have already been obtained. New fast quantum algorithms have been proposed [31-35]. Error correction techniques [10,27,31,36,37], unitary operations corresponding to the simplest logic gates [5-30], and some Hamiltonians for gate operation [10,14,24,28-30] have been explored. Ideas on how to combine the simplest quantum gates have been put forth, e.g., [7,15,38]. Experimentally, there are several atomic-scale systems where the simplest quantum-gate functions have been recently realized [26,39,40] or contemplated [19].

There remain, however, many conceptual difficulties with "macroscopic" quantum computing [4,18]. For instance, the reversibility of coherent quantum evolution implies that the time scale Δt of the operation of quantum logic gates must be built into the Hamiltonian. As a result, virtually all proposals available to date assume that computation will be externally timed, i.e., interactions will be switched "on" and "off," for instance, by laser radiation. Thus, while we recognize that eventually quantum behavior on the atomic scale will have to be considered in computer component design, we also accept that it is still a long way to go, with modern technology, to a really macroscopically coherent quantum computational unit.

In this work we therefore adopt a more realistic view that technological advances might first allow design and manufacturing of limited-size units, based on several tens of atomic two-level systems, operating in a quantum-coherent fashion over a sufficiently large time interval to function as parts of a larger "classical" computer which will not maintain a quantum-coherent operation over its macroscopic dimensions.

We have initiated study of the simplest quantum logic gates in order to identify which interaction terms are typical in Hamiltonians required for their operation. Results presently available are limited; they include Hamiltonians for certain NOT [14,28] and controlled-NOT gates [10,30], and for some copying processes [29,30], as well as general analyses of possibility of construction of quantum operations [8,22].

In order to make connections with the present "classical" computer-circuitry design and have a natural way of identifying, at least initially, which multi-qubit systems are of interest, we propose to consider spatially extended quantum gates, i.e., gates with input and output qubits different. Our goal is to be able to "design" interaction parameters, presumably by numerical simulations, to have such gates perform useful Boolean operations. In this work we carry out such a "design" analytically for the three-spin XOR gate; one special-case result of this work was reported in a short publication [41]. Incorporating "designed" coherent

computational units in a larger classical computer will require a whole new branch of computer engineering because the "built-in" Boolean functions will be complicated as compared to the conventional NOT, AND, OR, NAND, etc., to which computer designers are accustomed. Furthermore, the rules of their interconnection with each other and with the rest of the classical computer will be different from today's devices.

Reversibility of coherent quantum evolution makes the distinction between the input and output less important than in irreversible computer components. However, we consider the notion of separate (or at least not necessarily fully identical) input and output useful within our general goals: to learn what kind of interactions are involved and to consider also units that might be connected to/as in "classical" computer devices. While our present study is analytical, we foresee numerical studies of systems of order 20 to 25 two-state (qubit) atomic "components" with variable general-parameter interactions.

The outline of this work is as follows. In Section 2, we define the problem and introduce some notation. In Section 3, we analyze the matrix forms of the unitary evolution operator and Hamiltonian operator. The latter is explicitly calculated in Section 4 and then further refined in Sections 4 and 5 to yield a two-spin-interaction result.

2. The Three-Spin XOR Gate

We will use the term "spin" to describe a two-state system, and we will represent spin-$\frac{1}{2}$-particle spin-components (measured in units of $\hbar/2$) by the standard Pauli matrices $\sigma_{x,y,z}$. In Figure 1, we denote by A, B, C the three two-state systems, i.e., three spins, involved. We assume that at time t the input spins A and B are in one of the basis states $|AB\rangle = |11\rangle$, $|10\rangle$, $|01\rangle$, or $|00\rangle$, where 1 and 0 denote the eigenstates of the z-component of the spin operator, with 1 referring to the "up" state and 0 referring to the "down" state. We use this notation for consistency with the classical "bit" notion. The initial state of C is not specified (it is arbitrary).

We would like to have a quantum evolution which, provided A and B are initially in those basis states, mimics the XOR function:

A	B	output
1	1	0
1	0	1
0	1	1
0	0	0

(2.1)

were the output is at time $t + \Delta t$. One way to accomplish this is to produce the output in A or B, i.e., work with a two-spin system where the input and output are the same. The Hamiltonian for such a system

is not unique. Explicit examples can be found in [10,30] where XOR was obtained as a sub-result of the controlled-NOT gate operation. In this case of two spins involved, the interactions can be single- and two-spin only.

An important question is whether multispin systems can produce useful logical operations with only two-spin and, for larger systems, short-range interactions. Indeed, short-range two-particle interactions are much better studied and accessible to experimental probe than multiparticle interactions. Here we require that the XOR result be put in C at time $t+\Delta t$; see Figure 1. The final states of A and B, as well as the *phase* of C are arbitrary. In fact, there are many different unitary transformations, U, that correspond to the desired evolution in the eight-state space with the basis $|ABC\rangle = |111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle$, which we will use in this order. The choice of the transformation determines what happens when the initial state is a superposition of the reference states, what are the phases in the output, etc.

Let us consider first, for illustration, the following Hamiltonian [41]

$$H = \frac{\pi\hbar}{4\Delta t}\left(\sqrt{2}\sigma_{zA}\sigma_{yB} + \sqrt{2}\sigma_{zB}\sigma_{yC} - \sigma_{yB}\sigma_{xC}\right) \qquad (2.2)$$

It is written here in terms of the spin components; the subscripts A, B, C denote the spins. In the eight-state basis specified earlier, its matrix

can be obtained by direct product of the Pauli matrices and unit 2×2 matrices $\mathcal{I}$. For instance, the first interaction term is proportional to

$$\sigma_{zA} \otimes \sigma_{yB} \otimes \mathcal{I}_C \tag{2.3}$$

etc. This Hamiltonian involves only two-spin-component interactions. In fact, in this particular example A and C only interact with B.

One can show that the Hamiltonian (2.2) corresponds to the XOR result in C at $t+\Delta t$ provided A and B where in one of the allowed superpositions of the appropriate "binary" states at t (we refer to superposition here because C is arbitrary at t). There are two ways to verify this [41]. Firstly, one can diagonalize H and then calculate the unitary evolution operator (matrix) U in the diagonal representation by using the general relation (valid for Hamiltonians which are constant during the time interval Δt; see [28] for a formulation that introduces a multiplicative time dependence in H),

$$U = \exp\left(-iH\Delta t/\hbar\right) \tag{2.4}$$

and then reverse the diagonalizing transformation. The calculation is quite cumbersome.

The second, more general approach adopted here is to "design" a

whole family of two-spin-interaction Hamiltonians of which the form (2.2) is but a special case, by analyzing generally a family of 8×8 unitary matrices corresponding to the XOR evolution. This "design" program is carried out in the following sections.

3. The Structure of the Unitary Matrix and Hamiltonian

We require any linear combination of the states $|\underline{1}\underline{1}1\rangle$ and $|\underline{1}\underline{1}0\rangle$ to evolve into a linear combination of $|11\underline{0}\rangle$, $|10\underline{0}\rangle$, $|01\underline{0}\rangle$, and $|00\underline{0}\rangle$, compare the underlined quantum numbers with the first entry in (2.1), with similar rules for the other three entries in (2.1).

In the matrix notation, and in the standard basis introduced earlier, namely, $|ABC\rangle = |111\rangle, |110\rangle, |101\rangle, |100\rangle, |011\rangle, |010\rangle, |001\rangle, |000\rangle$, the most general XOR evolution operator corresponding to the Boolean function (2.1), with the output in C, is, therefore,

$$U = \begin{pmatrix} 0 & 0 & U_{13} & U_{14} & U_{15} & U_{16} & 0 & 0 \\ U_{21} & U_{22} & 0 & 0 & 0 & 0 & U_{27} & U_{28} \\ 0 & 0 & U_{33} & U_{34} & U_{35} & U_{36} & 0 & 0 \\ U_{41} & U_{42} & 0 & 0 & 0 & 0 & U_{47} & U_{48} \\ 0 & 0 & U_{53} & U_{54} & U_{55} & U_{56} & 0 & 0 \\ U_{61} & U_{62} & 0 & 0 & 0 & 0 & U_{67} & U_{68} \\ 0 & 0 & U_{73} & U_{74} & U_{75} & U_{76} & 0 & 0 \\ U_{81} & U_{82} & 0 & 0 & 0 & 0 & U_{87} & U_{88} \end{pmatrix} \tag{3.1}$$

The condition of unitarity, $UU^\dagger = 1$, reduces the number of independent parameters. Still they are too numerous for the problem to be manageable analytically; recall that each nonzero element U_{kn} is complex and therefore involves two real parameters. Thus, we are going to consider a subset of operators of the form (3.1).

From our earlier work [28] we know that one convenient way to reduce the number of parameters and at the same time ensure automatic unitarity is to have a single phase factor in each column and row of the matrix. Furthermore, we choose a form which is diagonal in the states of the A-spin,

$$U = \begin{pmatrix} V_{4\times4} & 0_{4\times4} \\ 0_{4\times4} & W_{4\times4} \end{pmatrix} \tag{3.2}$$

Thus, A and B are not treated symmetrically. Here $0_{4\times4}$ denotes the 4×4 matrix of zeros. The 4×4 matrices V and W are parametrized as follows:

$$V = \begin{pmatrix} 0 & 0 & e^{i\delta} & 0 \\ e^{i\alpha} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{i\beta} \\ 0 & e^{i\gamma} & 0 & 0 \end{pmatrix} \tag{3.3}$$

$$W = \begin{pmatrix} 0 & e^{i\rho} & 0 & 0 \\ 0 & 0 & 0 & e^{i\omega} \\ e^{i\xi} & 0 & 0 & 0 \\ 0 & 0 & e^{i\eta} & 0 \end{pmatrix} \tag{3.4}$$

The reasons for this choice of an 8-parameter unitary matrix U will become apparent in the course of the calculation. Some of the features can be explained at this stage as follows. We note that, omitting the direct-product symbols and replacing unit matrices by 1, etc., the matrix U in (3.2) has the structure

$$2U = (1 + \sigma_{zA})\, V + (1 - \sigma_{zA})\, W = V + W + \sigma_{zA}(V - W) \qquad (3.5)$$

where V and W are operators in the space of B and C. Since U was chosen diagonal in the space of A, the Hamiltonian, H, will have a similar structure,

$$2H = P + Q + \sigma_{zA}(P - Q) \qquad (3.6)$$

with the appropriate $(B \otimes C)$-space Hamiltonians P and Q. Now in order to avoid three-spin interactions, $P - Q$ must be linear in Pauli matrices. On the other hand, we also prefer to avoid single-spin (external-field) interactions. Thus, $P + Q$ must contain only terms of the second order in the spin components while $P - Q$ must contain only terms of the first order in the spin components. This suggests avoiding putting phase factors on the diagonal, which would lead to matrices similar to those encountered in extended-NOT-gate calculations [28] that are known to be of a structure undesirable here: they contain a mixture of first-order and second-order

terms. The off-diagonal choices remaining are considerably limited; the forms (3.3) and (3.4) are thus nearly unique.

In summary, while the arguments are admittedly vague and they do involve a certain level of guess, trial and error, the presented parametrization offers a good chance that with further restrictions on the parameters a two-spin interaction Hamiltonian can be obtained. As will be seen later, five conditions are imposed so that the resulting Hamiltonian depends on three (real) parameters.

4. The Hamiltonian Matrix

Let us define

$$\mu = \frac{\alpha + \beta + \gamma + \delta}{4} \tag{4.1}$$

$$\nu = \frac{\rho + \omega + \xi + \eta}{4} \tag{4.2}$$

and also introduce the reduced operators p and q according to

$$P = -\frac{\hbar}{\Delta t}p \quad \text{and} \quad Q = -\frac{\hbar}{\Delta t}q \tag{4.3}$$

Then (2.4) reduces to

$$V = \exp(ip) \quad \text{and} \quad W = \exp(iq) \tag{4.4}$$

The following calculations are rather cumbersome. Only the results will be presented. The algebraic steps omitted are straightforward. First, we diagonalize V and W: we calculate their eigenvalues and also the matrices of their normalized eigenvectors. The latter can be used to transform to the diagonal representations.

Specifically, the eigenvalues of V are $e^{i\mu}$, $ie^{i\mu}$, $-e^{i\mu}$, $-ie^{i\mu}$. The appropriate eigenvalues of p then follow form (4.4) as μ, $\mu + \frac{1}{2}\pi$, $\mu + \pi$, $\mu + \frac{3}{2}\pi$. Arbitrary multiples of 2π can be added to these choices. However, there are certain nonrigorous arguments in the literature [28] for generally keeping the spread of eigenvalues of the Hamiltonian as small as possible. Thus, we choose the simplest expressions. The eigenvalues of q are determined identically, with μ replaced by ν throughout.

The next step is to apply the inverse of the diagonalizing transformations for V and W to the diagonal 4×4 matrices for, respectively,

p and q. The latter contain the eigenvalues of p and q as the diagonal elements. The results are the matrix forms of the operators p and q in the original representation:

$$\frac{4}{\pi}p = \begin{pmatrix} \frac{4}{\pi}\mu + 3 & -(1+i)e^{i(\mu-\alpha)} & -(1-i)e^{i(\delta-\mu)} & -e^{i(2\mu-\alpha-\gamma)} \\ -(1-i)e^{i(\alpha-\mu)} & \frac{4}{\pi}\mu + 3 & -e^{i(2\mu-\beta-\gamma)} & -(1+i)e^{i(\mu-\gamma)} \\ -(1+i)e^{i(\mu-\delta)} & -e^{i(\beta+\gamma-2\mu)} & \frac{4}{\pi}\mu + 3 & -(1-i)e^{i(\beta-\mu)} \\ -e^{i(\alpha+\gamma-2\mu)} & -(1-i)e^{i(\gamma-\mu)} & -(1+i)e^{i(\mu-\beta)} & \frac{4}{\pi}\mu + 3 \end{pmatrix} \quad (4.5)$$

$$\frac{4}{\pi}q = \begin{pmatrix} \frac{4}{\pi}\nu + 3 & -(1-i)e^{i(\rho-\nu)} & -(1+i)e^{i(\nu-\xi)} & -e^{i(\rho+\omega-2\nu)} \\ -(1+i)e^{i(\nu-\rho)} & \frac{4}{\pi}\nu + 3 & -e^{i(\omega+\eta-2\nu)} & -(1-i)e^{i(\omega-\nu)} \\ -(1-i)e^{i(\xi-\nu)} & -e^{i(2\nu-\omega-\eta)} & \frac{4}{\pi}\nu + 3 & -(1+i)e^{i(\nu-\eta)} \\ -e^{i(2\nu-\rho-\omega)} & -(1+i)e^{i(\nu-\omega)} & -(1-i)e^{i(\eta-\nu)} & \frac{4}{\pi}\nu + 3 \end{pmatrix} \quad (4.6)$$

As expected, the resulting matrices are Hermitean.

5. The Two-Spin-Interaction XOR Hamiltonian

Thus far we decreased the number of independent parameters in the general unitary transformation and chose it to be diagonal in the A-space. We now "refine" our design of the Hamiltonian to favor interaction of the second order in the Pauli matrices. First, we note that both P and Q are constant-diagonal matrices. In terms of the Pauli matrices, then, both their sum and difference in (3.6) will involve constant terms. These are undesirable because in $\sigma_{zA}(P-Q)$ they lead to terms of order one (instead of the desired two), in H, while in $P+Q$ they lead to an additive constant in H which only affects the overall phase of the unitary transformation and is of no interest otherwise. Therefore, we put

$$\mu = \nu = -\frac{3}{4}\pi \tag{5.1}$$

in order to nullify these diagonal elements in both P and Q.

Let us now focus our attention on $P - Q$ which, by (5.1), is now a matrix with zero diagonal. We must impose conditions on the parameters to make $P - Q$ of order exactly one in the Pauli matrices. We note, however, that due to zero-diagonal, it cannot contain σ_z terms. The general form liner in σ_x, σ_y is

$$P-Q=\mathcal{I}_B\otimes\begin{pmatrix}0 & X\\ X^* & 0\end{pmatrix}_C+\begin{pmatrix}0 & Y\\ Y^* & 0\end{pmatrix}_B\otimes\mathcal{I}_C=\begin{pmatrix}0 & X & Y & 0\\ X^* & 0 & 0 & Y\\ Y^* & 0 & 0 & X\\ 0 & Y^* & X^* & 0\end{pmatrix} \tag{5.2}$$

where the stars denote complex conjugation, X and Y are arbitrary (complex) numbers, and $\mathcal{I}$ stands for the unit matrix as before. Thus we require that $P-Q$ be of the form suggested by (5.2). This imposes several rather cumbersome algebraic conditions: two above-diagonal elements of the difference must be equal to zero while the remaining four elements must be equal pairwise. After a lengthy but straightforward algebra not reproduced here, we conclude that these conditions can be satisfied if α, β, γ are kept as three independent (real) parameters while the remaining angles are given by

$$\delta = -3\pi - \alpha - \beta - \gamma \tag{5.3}$$

$$\rho = -\pi + \beta \tag{5.4}$$

$$\omega = -2\pi - \alpha - \beta - \gamma \tag{5.5}$$

$$\xi = -\pi + \gamma \tag{5.6}$$

$$\eta = \pi + \alpha \tag{5.7}$$

These conditions take care of the form of $P-Q$. Interestingly, our results below also show that $P+Q$ contains only two-spin interactions with this choice of parameters. We have no simple explanation of this property (of the absence of first-order terms in $P+Q$). It is probably related to the fact that the structure pattern of the original matrices V and W is quite similar even though the precise positioning of nonzero elements in them is different. Note that (5.1) is built into (5.3)-(5.7). The explicit expressions are obtained by a lengthy calculation,

$$P+Q=-\frac{\sqrt{2}\pi\hbar i}{4\Delta t}\times$$

$$\begin{pmatrix} 0 & e^{-i\alpha}+e^{i\beta} & e^{-i(\alpha+\beta+\gamma)}-e^{-i\gamma} & -\sqrt{2}e^{-i(\alpha+\gamma)} \\ -e^{i\alpha}-e^{-i\beta} & 0 & -\sqrt{2}e^{-i(\beta+\gamma)} & e^{-i\gamma}-e^{-i(\alpha+\beta+\gamma)} \\ e^{i\gamma}-e^{i(\alpha+\beta+\gamma)} & \sqrt{2}e^{i(\beta+\gamma)} & 0 & -e^{-i\alpha}-e^{i\beta} \\ \sqrt{2}e^{i(\alpha+\gamma)} & e^{i(\alpha+\beta+\gamma)}-e^{i\gamma} & e^{i\alpha}+e^{-i\beta} & 0 \end{pmatrix} \tag{5.8}$$

$$P-Q=-\frac{\sqrt{2}\pi\hbar i}{4\Delta t}\times$$

$$\begin{pmatrix} 0 & e^{-i\alpha}-e^{i\beta} & e^{-i(\alpha+\beta+\gamma)}+e^{-i\gamma} & 0 \\ -e^{i\alpha}+e^{-i\beta} & 0 & 0 & e^{-i(\alpha+\beta+\gamma)}+e^{-i\gamma} \\ -e^{i(\alpha+\beta+\gamma)}-e^{i\gamma} & 0 & 0 & e^{-i\alpha}-e^{i\beta} \\ 0 & -e^{i(\alpha+\beta+\gamma)}-e^{i\gamma} & -e^{i\alpha}+e^{-i\beta} & 0 \end{pmatrix} \tag{5.9}$$

Finally, we expand these matrices in terms of products of the Pauli matrices and collect terms according to (3.6) to get

$$H = -\frac{\pi\hbar}{8\Delta t}\Big\{\sqrt{2}\,(\sin\alpha+\sin\beta)\,\sigma_{zA}\sigma_{xC} - \sqrt{2}\,(\cos\alpha-\cos\beta)\,\sigma_{zA}\sigma_{yC}$$

$$+\sqrt{2}\big[\sin\gamma+\sin(\alpha+\beta+\gamma)\big]\sigma_{zA}\sigma_{xB} - \sqrt{2}\big[\cos\gamma+\cos(\alpha+\beta+\gamma)\big]\sigma_{zA}\sigma_{yB}$$

$$+\sqrt{2}\,(\sin\alpha-\sin\beta)\,\sigma_{zB}\sigma_{xC} - \sqrt{2}\,(\cos\alpha+\cos\beta)\,\sigma_{zB}\sigma_{yC}$$

$$-\sqrt{2}\big[\sin\gamma-\sin(\alpha+\beta+\gamma)\big]\sigma_{xB}\sigma_{zC} + \sqrt{2}\big[\cos\gamma-\cos(\alpha+\beta+\gamma)\big]\sigma_{yB}\sigma_{zC}$$

$$-\big[\sin(\alpha+\gamma)+\sin(\beta+\gamma)\big]\sigma_{xB}\sigma_{xC} + \big[\cos(\alpha+\gamma)-\cos(\beta+\gamma)\big]\sigma_{xB}\sigma_{yC}$$

$$+\big[\cos(\alpha+\gamma)+\cos(\beta+\gamma)\big]\sigma_{yB}\sigma_{xC} + \big[\sin(\alpha+\gamma)-\sin(\beta+\gamma)\big]\sigma_{yB}\sigma_{yC}\Big\} \tag{5.10}$$

Note that (2.2) corresponds to the parameter choice $\alpha = \beta = \gamma = 0$. The Hamiltonian (5.10) describes the three-spin XOR for arbitrary parameter values. All the interactions involved are two-spin as desired. The result, however, is not symmetric in any obvious way. It seems to correspond to complicated tensor interactions involving expressions of order two in the components of the three spins involved. No rotational or other symmetry in the three-component spin space, or planar symmetry, or uniaxial coupling, are apparent. All these would correspond to the familiar Heisenberg, XY, and Ising couplings in condensed matter physics.

Thus, in order to realize interaction (5.10) in materials, a rather anisotropic medium with highly nonsymmetric tensorial magnetic interactions will be required. In this respect our analytical attempt to "design" a

multi-spin quantum gate in this work may indicate that different roots to the derivation of Hamiltonians should be also explored. One should start with the more conventional magnetic interactions, isotropic (Heisenberg), planar (XY), uniaxial (Ising), write down general-parameter Hamiltonians, and then adjust the coupling parameters numerically in search of those values for which useful Boolean gate operations are carried out. There is no guarantee that such a program will succeed. We intend to pursue both approaches in our future work.

In summary, we derived a three-parameter family of Hamiltonians that correspond to the three-spin XOR gate. While our calculation demonstrates that multi-spin gates can accomplish quantum-logic operations with two-particle, short-range interactions, our results seem also to call for further work seeking improvement in two ways. Firstly, our derivation is not general and it has involved a good deal of guesswork. Secondly, the terms in the resulting Hamiltonians have no obvious grouping by symmetries.

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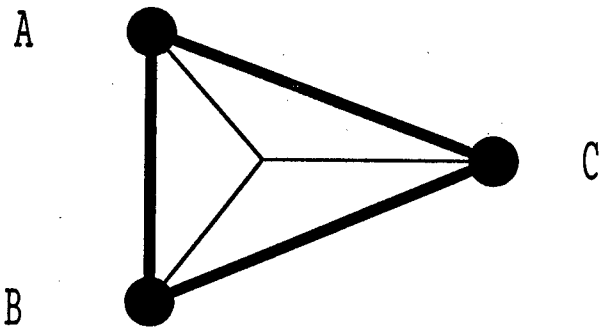

Figure 1: Three two-state systems (spins) A, B, C, with the pairwise spin-component interactions marked schematically by the connecting thick lines. The XOR operation accomplished in time Δt assumes that A and B are the input qubits and C is the output qubit. The goal is to avoid multi-spin interactions; here these are the three-spin interactions marked schematically by the thin lines.

Chapter 2

Quantum Computing Using Electron-Nuclear Double Resonances

This section was published as a paper in: *Photonic Quantum Computing*, S.P. Hotaling and A.R. Pirich, editors, SPIE Press vol. 3076, 1997. Hence, the present section is a preprint of that paper. This paper summarizes earlier experimental work by Hotaling (cf. 1995).

Quantum computing using electron-nuclear double resonances

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ABSTRACT

We consider the use of Electron-Nuclear Double Resonance (ENDOR) techniques in quantum computing. ENDOR resolution as a possible limiting factor is discussed. It is found that ENDOR and double-ENDOR techniques have sufficient resolution for quantum computing applications.

Key Words: Quantum Computing, Nuclear Magnetic Resonance, Electron Nuclear Double Resonance

1. INTRODUCTION

Recently, one of the authors presented arguments that the Electron Nuclear Double Resonance (ENDOR) process may be exploited for the storage and processing of discrete data on a quantum scale[1–6]. The implication is that a solid state realization of a quantum mechanical computer could be engineered. Among the advantages are that such a solid state quantum computer would be stable, programmable, and input/output (I/O) controllable by current state-of-the-art technology. It could be envisioned, in principle, to be engineerable for considerably lower per unit cost than quantum computers operating on the principle of induced quantum superposition and entangled states of trapped ions[7], or photon states using microcavities[8]. Furthermore, solid state ENDOR is a well established procedure (established by Feher[9] in 1959), and laboratory components are commercially available at reasonable costs. The present paper is a proposed novel quantum computing paradigm based upon the use of multipulse resonance techniques to manipulate nuclear spins of a mostly relatively low dimensional ensemble deviation from thermal equilibrium[10]. The new paradigm builds upon a previously proposed paradigm which utilizes well established techniques from nuclear magnetic resonance (NMR) spectroscopy[11]. An obvious advantage to using superposition of nuclear spins for quantum logic gates, and nuclear spin flips to conduct quantum computing, is the possibility of extraordinary long decoherence times due to the relative isolation of nuclear spins within a molecule. A disadvantage is related to this, and that is the length of time required to couple information in and out of a system and manipulation during computation. Another disadvantage is that nuclear spin flips are induced at radio frequency (rf) wavelengths, and so quantum computation is restricted to temporal unitary evolution and is entirely non-local.

In the present paper, we propose a scheme based upon Electron Nuclear Double Resonance (ENDOR) as a means to practical quantum computation. The proposed scheme builds from the previous proposals which use NMR spectrographic techniques[10,11], but trades reduction in decoherence time by electron spin, nuclear spin coupling, but gains in high I/O bit rates and stronger coupling to manipulate computation. Also, we shall point out that sequential spatially dependent architecture is possible using laser electronic excitation to manipulate electron spin coupling to nuclear spins.

A brief discussion of Electron Spin Resonance (ESR) and ENDOR will be presented in the next section. Our novel paradigm for quantum computing using laser-induced electronic excitation and ENDOR will be discussed in Section 3, and Section 4 will be used for summary and conclusion.

2. ESR AND ENDOR BACKGROUND

The theory of ESR is derivable from the Dirac theory and will not be treated here, but may be found in the literature[1–6, 9, 12–13]. Here, we simply state the essential spin Hamiltonian and discuss its interaction terms,

$$\mathcal{H} = \beta \mathbf{H} \cdot \mathbf{g} \cdot \mathbf{S} - \beta_N \mathbf{H} \cdot \mathbf{g}_N \cdot \mathbf{I} + \lambda \mathbf{L} \cdot \mathbf{S} + \mathbf{S} \cdot \mathbf{A} \cdot \mathbf{I}. \quad (1)$$

The first and second terms correspond to the Zeeman energy contributions due to the electron sin, **S**, and nuclear spin, **I**, coupling to the magnetic field **H**. Here, **g** is the coupling tensor in units of the Bohr magneton β and $\mathbf{g}_N$ is the nuclear spin coupling tensor in units of the nuclear magneton, β_N. The third term in the Hamiltonian is the Zeeman interaction associated with the coupling between the magnetic moment due to the electrons intrinsic spin and that due to the electrons orbital momentum in a bound state. This term contains information about electronic defect states with different microscopic properties through measurement of shifts in g-value of a paramagnetic site. The last term is the hyperfine term which expresses the magnetic interaction between the nuclear and electronic spins due to overlap of the electronic wave functions with nuclear spins. This term, governed by the interaction tensor **A**, depends upon nuclear spin contact interaction with electronic wave functions and can be nearly isotropic, as with nearly s-type electronic orbitals, or anisotropic as for p- or d-like orbitals. By analyzing the energy contributions in the hyperfine term, the nature of the spin center (type of electronic state) can be determined.

Electron Nuclear Double Resonance (ENDOR) provides the capability to more closely examine the anisotropic hyperfine interaction in terms of the atomic and electronic interactions at the paramagnetic centers. Ions or free radicals trapped in a solid lattice experience perturbations in their energy levels as expressed by this matrix. These perturbations can affect the spin transition dynamics of the paramagnetic species, and be detectable by Electron Spin Resonance (ESR). ENDOR allows the hyperfine and spin lattice relaxation phenomena to be measured by detecting the Nuclear Magnetic Resonance (NMR) signal as a change in the ESR spectrum.

In ENDOR, the nuclear spins are modulated by addition of a transverse rf field, while the electron spins are driven by a transverse microwave (MW) field. The main aspects of the ENDOR process can be illustrated by the simplified version of Eq. (1),

$$\mathcal{H} = g\beta H_0 S_z + a\, \mathbf{S} \cdot \mathbf{I} - g_N \beta_N H_0 I_z, \quad (2)$$

where we have neglected spin-orbit coupling, which in many cases is quenched[12]. The eigenenergies associated with $\mathcal{H}$, Eq. (2), in terms of the appropriate quantum numbers are given by

$$E(m_S, m_I) = g\beta H_0 m_S + a\, m_S m_I, \quad (3)$$

where we assume that the electronic Zeeman energy, given by the first term, and the hyperfine energy, the second term in Eq. (3), are much larger than the nuclear Zeeman energy. The corresponding energy level structure, together with the ordering of the energy levels and transitions in terms of the quantum numbers is illustrated in Fig. 1. Provided $\delta \neq 0$, transitions $|4\rangle \rightarrow |2\rangle$ and $|3\rangle \rightarrow |1\rangle$ cause simultaneous electron-nuclear double spin flips at the transition energy $\hbar\omega = 2\Delta$. Whereas, transitions $|4\rangle \rightarrow |1\rangle$ and $|3\rangle \rightarrow |2\rangle$ correspond to electron spin flips only, but at the transition energy $\hbar\omega = 2\Delta + 2\delta$. The usual ENDOR procedure requires that the electronic transition be saturated using a microwave field at frequency $\omega = 2\Delta/\hbar$; then nuclear spin flips are induced with an rf field at frequency $\Omega = 2\delta/\hbar$ and appear as modifications in the electron spin-resonance spectrum.

To date, the most prevalent application of the ESR process in solid state materials is the determination and characterization of defect structures. As discussed above, the hyperfine interaction between the magnetic moments of an unpaired electron and neighboring nuclei can yield this information. The hyperfine interaction is sometimes not well resolved due to lattice phonon modes. This is especially true of the super-hyperfine interaction or ligand hyperfine interaction which appears in the ESR spectrum as an interaction between the magnetic moment of an unpaired electron spin and its nearest neighbor nuclei. To the untrained eye, this broadening effect appears as a fundamental resolution limitation of magnetic resonance techniques. However, in the ENDOR process, the NMR transitions of neighboring nuclei interacting with the unpaired electron spin are measured by detecting their influence on the unpaired spins polarization under favorable signal-to-noise experimental conditions (partially saturated spin-resonance condition). These ENDOR-detected NMR transitions are detected as quantum

$$H = g\,\beta\,H_0\,S_z + a\,S \bullet I - g_n\,\beta_n\,H_0\,I_z$$

$$E(m_S, m_I) = g\,\beta\,H_0\,m_S + a\,m_S\,m_I$$

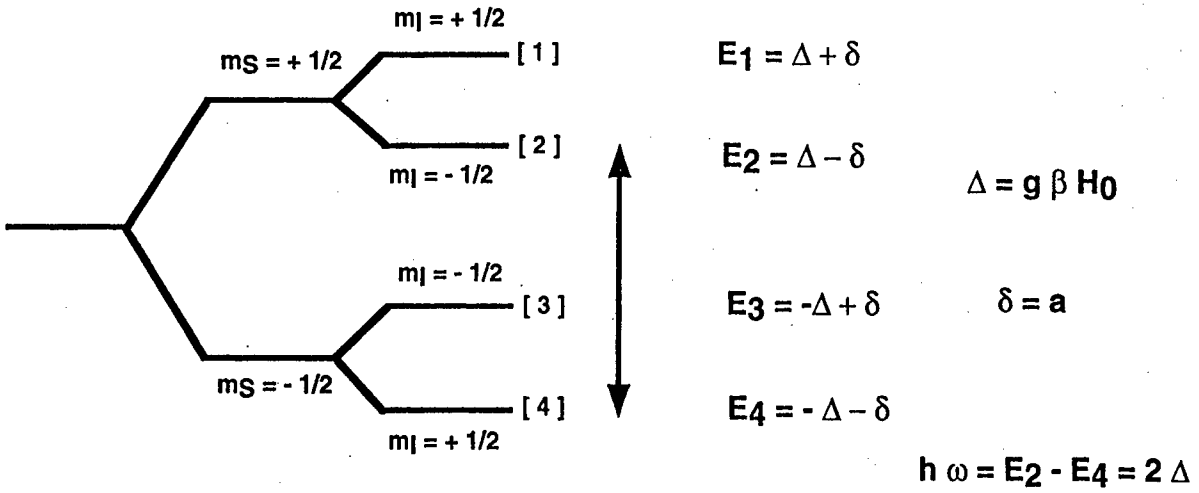

Fig.1 Energy level structure and transitions from Equ. (1).

mechanical transitions of much higher energy than would be observed in conventional NMR or ESR techniques. This implies that there are far fewer lines in the ENDOR spectrum to resolve than in the conventional ESR or NMR spectra. This is shown schematically in Figure 2 for the spin 1/2 system where we note that the ENDOR transition (cross transition) is larger than, and fewer in number than, either the ESR or NMR transitions. The effect is more noticeable for higher order spin systems (I = 3/2, ..., etc.). This enhancement has been reported experimentally in SrFCl and BaFCl systems[14–16].

A strong advantage associated with the paradigm presented here is the possibility to control the transferred hyperfine interaction, the tensor A in Eq. (1), used as a generic example and illustrated in Fig. 3a. Here, an unpaired electron orbital associated with atom, A, is represented as an s-state in the electronic ground state, without any overlap of the wave function at the nucleus of atom, B. Laser excitation of atom, A, on the other hand, induces an electronic transition to a p-orbital or d-orbital, with consequent overlap of the electron wave function at the nucleus, B, inducing S_A, I_B electron spin, nuclear spin interaction, as shown in Fig. 3b. If a microwave field is tuned to the transition shown in Fig. 1, a simultaneous electron spin S_A, nuclear spin, I_B, transition, double spin flip is induced Thus, nuclear spin flips can be controlled in atom, B, by electron spin flips controlled by laser-induced transferred hyperfine interaction[17].

This scheme constitutes a significant modification of the NMR quantum computation of Refs. 10–11. Here, we use that paradigm to build a controlled NOT-gate conditional on a reference nuclear spin, but introduce laser field-induced electron spin, nuclear spin coupling by laser-induced transferred Fermi contact interaction. Thus, input/output and control can be executed locally under unitary time evolution, $U = \exp[-i\,\mathcal{H}\,\Delta t/\hbar]$, and the laser field can be used to induce π-pulse excitation/de-excitation of duration Δt in subpicosecond time scale. Thus, decoherence can be minimized and control can be executed on the ultrafast time scale. In essence, we trade off some decoherence for fast local control.

It is also possible to utilize Double-ENDOR (D-ENDOR) effects to increase the spectral resolution. In D-ENDOR, two NMR transitions are stimulated while the ESR transition is measured. In this case, typical improvements of a factor of 10:1 in resolution are obtained[18]. In addition, Optical Detected Magnetic Resonance (ODMR) has the potential for increased output resolution.

3. QUANTUM LOGIC CIRCUITS

Recently, quantum mechanical Hamiltonians for logic gate elements have been derived for: NOT[18], exclusive OR[19,20], and controlled-NOT (C-NOT)[10] operations. The former papers concerned theoretical derivations while in the latter paper by Gershenfeld and Chuang, NMR transitions were experimentally demonstrated to realize a C-NOT operation in hardware. This experiment, when taken along with earlier work[1–6,18–20], leads us to propose an ENDOR-based process paradigm for realization of higher complexity quantum logic gates.

Consider a spin system consisting of a free spin (electron or hole) in some photoactive crystal or polymer, its nearest neighbor nucleus B and its second nearest neighbor nucleus C, as illustrated in Figure 4. The magnetic moments of B and C are assumed distinct. Spin-spin interaction between S_A and I_B and S_A and I_C is defined by the anisotropic hyperfine tensor A [Eq. (1)]. Stimulating nuclei B and C by separate rf wavelengths ν_B and ν_C corresponding to NMR transition frequencies while simultaneously stimulating S_A by microwave radiation sets up a D-ENDOR system. Stimulation of S_A by external laser radiation, ν_L, serves as a control to flip the spin states of the D-ENDOR system. Alternately, I_B or I_C could be perturbed by IR lasers, but for simplicity, we assume only S_A laser stimulation. This controlled stimulation thus realizes a controlled NOT gate. Consider the spin interaction to be coupled to a chain of atoms (D, E, ..., N). Repeated pulsing of S_A would cause the quantum chain to respond as the quantum mechanical analog of a chain of emitters as shown in Figure 5. If N is even, then there is no net change in spin state at output, or |up⟩ → |up⟩. If N is odd, |up⟩ → |down⟩.

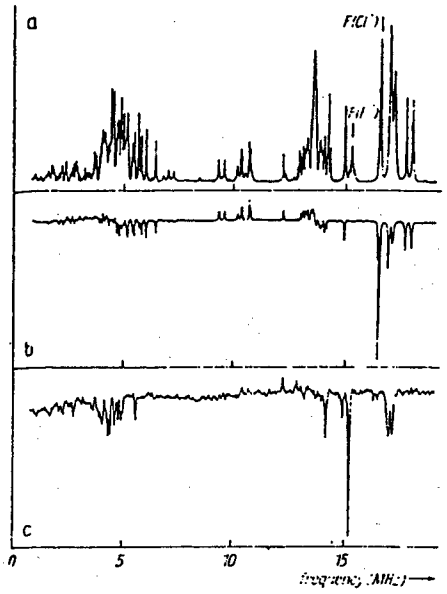

Fig. 2 a) Endor spectra of F(Cl⁻) and F(F⁻) centers in BaFCl for B_0 15⁰ off **c** in the **c**-**a** plane. b) Double ENDOR spectrum for setting f_1 to an ENDOR line of F(Cl) centers (see mark on Fig. 2a).

c) Double Endor spectrum for setting f_1 to an ENDOR line of F(F⁻) centers (see mark in Fig.2a).

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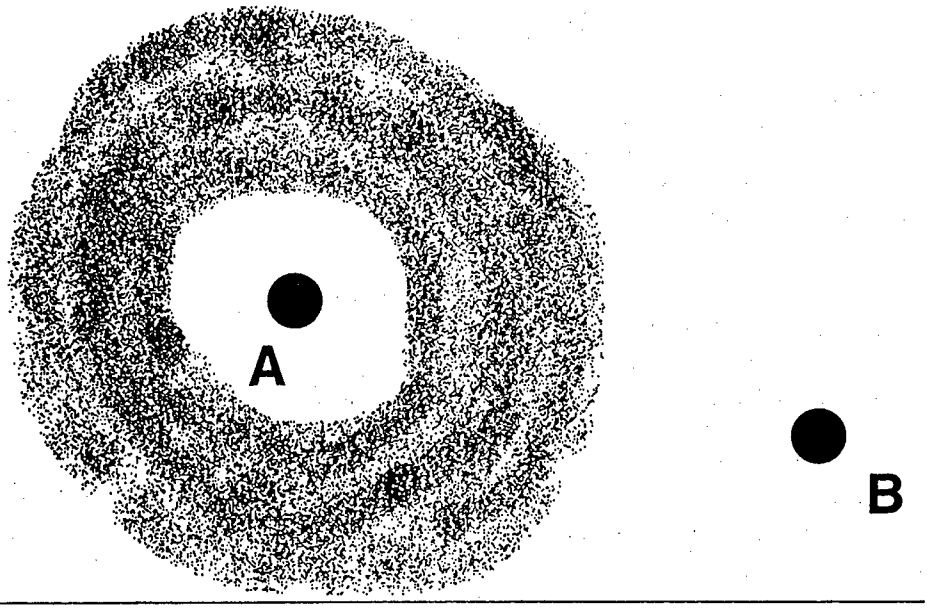

Fig. 3a Electronic S - state; A=0, ground state, no overlap.

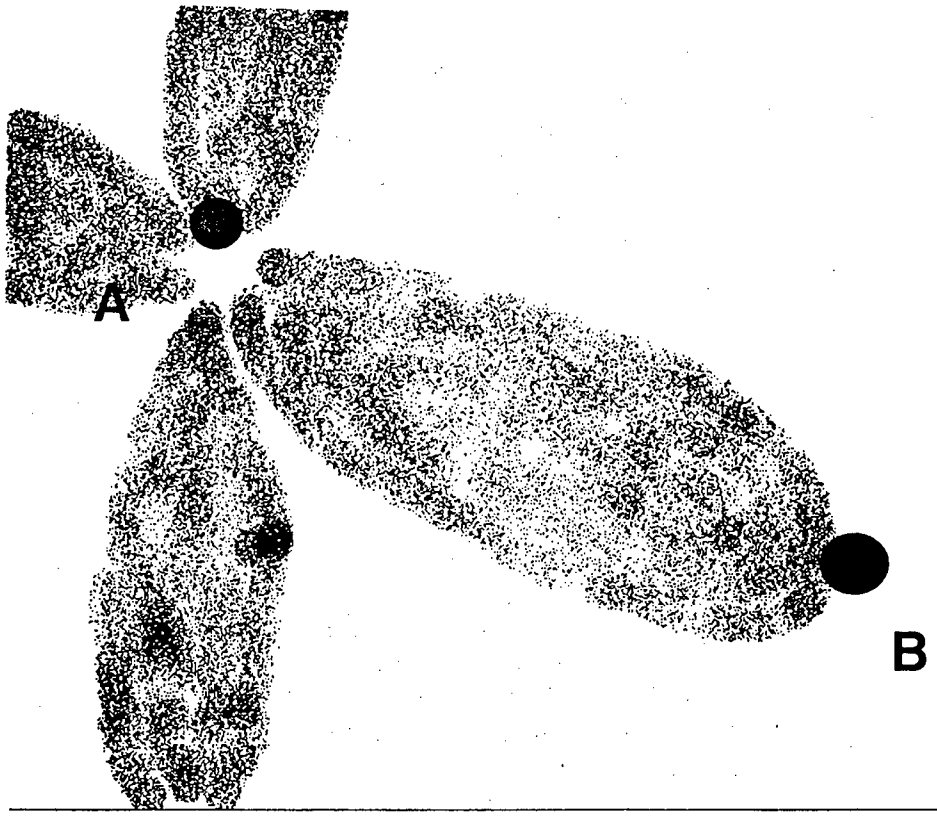

Fig. 3b Electronic p - state; A nonzero, excited state, overlap.

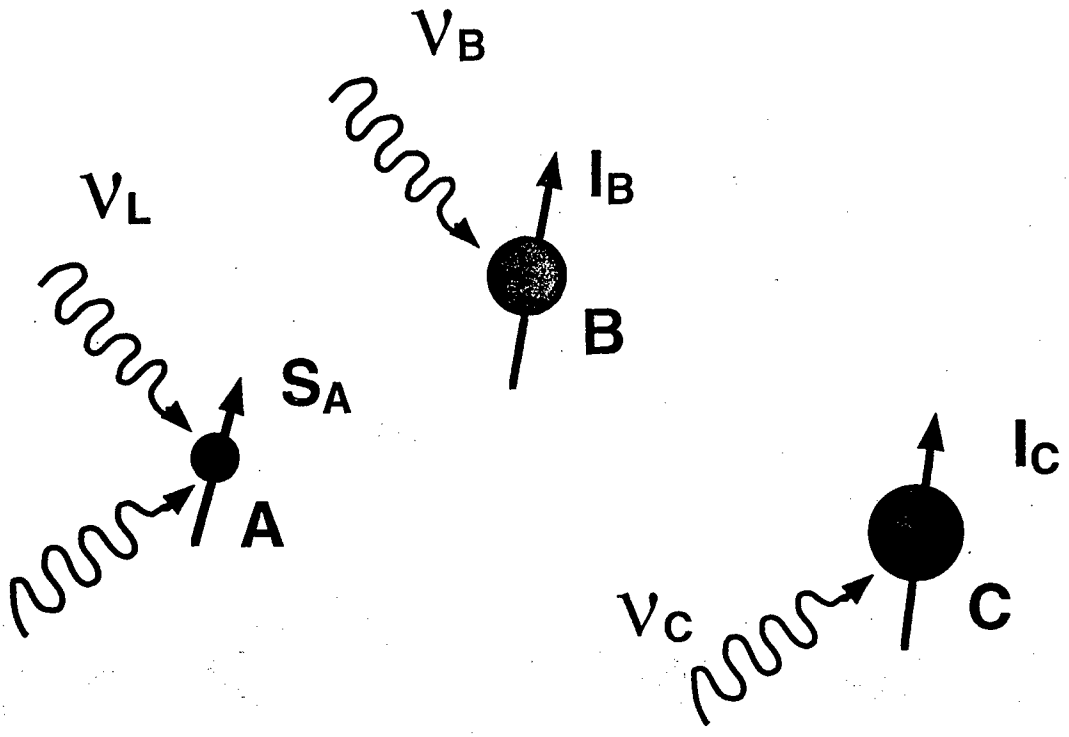

Fig. 4 Double ENDOR system; see text.

4. CONCLUSION

We have proposed a new paradigm for quantum computing which begins with the construction of a quantum controlled-NOT gate as prescribed in Reference 10, which uses a nonequilibrium ensemble of nuclear spins. The experiments of Gershenfeld, *et al.* have demonstrated exceptionally long decoherence times due to the relative isolation of nuclear magnetic moments to externally induced transitions. Our scheme introduces a higher-order process by coupling electron, nuclear double resonant superhyperfine transitions, controlled by laser-induced electronic transitions. The advantages of this scheme are that each complex molecule becomes, in and of itself, a quantum computer and the entire system represents massive parallelism. In addition, we have shown that laser-induced electronic excitation renders local control of gate preparation, spin flips, and input/output which can take place on the subpicosecond time scale. Here, we trade long decoherence times, intrinsic with nuclear spin flips, for controlled coupling with electron spin flips by transferred or superhyperfine interactions. The latter is regulated, i.e., on or off, by laser field π-pulse electron excitation/de-excitation. We hope that this will lead to near-term experimental investigations.

Fig. 5 Spin coupled to a chain of atoms; N even, no change at output, N odd, spin flip at output. Constitutes a controlled NOT gate.

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Chapter 3

Higher Radix Computation

Quantum mechanical systems are not limited to binary representation systems. Depending upon the atomic species under consideration, there may be many possible distinctly measurable excited states in addition to the ground state. This fact yields the possibility of designing a computational architecture with a radix exceeding 2. The possibility of having more than two distinct states also indicates the possibility of creating a logic machine with more than two truth values. Such a multivalued logic machine would have the potential for working in varied modal logics. Of course, we must recall the Russel-Whitehead thesis which proved that logic is distinct from arithmetic, but the possibility of nature providing the computer designer with such versatility is indeed intriguing at the least. The present chapter is a preprint of the author's paper on the subject of Radix R>2 quantum computing. The paper was published by the SPIE in 1997.

Radix-$R > 2$ Quantum Computation

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1 Abstract

A quantum mechanical system is presented for which a multiple-valued quantum algebra and logic are derivable. The system is distinguished from previous quantum computational proposals by the definition of higher order quantum algebras and logics derived from multi-level quantum spin systems.

2 Introduction

The potential impact and applications of quantum computing have recently been investigated by the community[1]. Most of the current literature considers quantum coherency to be of critical importance. This strict coherence constraint implies the necessity of isolated quantum systems which do not communicate with each other or the environment except at measurement (at which time the information content of the states is corrupted *vis.* the quantum measurement problem). The present work does not admit this constraint, allowing for mixed quantum states to encode and process information. The appeal of this relaxed constraint is that it may be possible to engineer a material system to perform quantum algebraic and logical operations in condensed matter systems at high temperatures, thus obviating the need to contain hundreds of ions in an ion trap at near-absolute zero temperatures.

3 A Simple Quantum Mechanical Finite State Machine

Consider a solid system rich in nuclear and electronic spin states (e.g. transition metal doped- $Bi_{12}SiO_{20}$ as used in Ref. [2]). A Spin Hamiltonian can be derived which allows for photonic perturbation of those electronic and nuclear spin states.[3]

Conjecture 1 *A finite state machine may be realized from spin states (corresponding to logic levels) in a condensed matter media and photonic perturbation (logical connectives) of those states.*

As a simple example of a multiple-valued quantum spin system, consider a system of two particles at fixed positions in space (separated by a distance r), endowed with spin $\frac{1}{2}$, and joined with unit vector $\mathbf{n}$. The state of the system is given by the state vector:

$$|\Psi\rangle = |S, I\rangle \tag{1}$$

where: S and I correspond to the spins, of the particles. The set $\{|s, i>\}$ is the basis of eigenvectors common to S_z and I_z (in the spin Hilbert space of spin states).

The magnetic moments of S and I are given by:

$$M_s = \gamma_s S \tag{2}$$

and

$$M_i = \gamma_i I \tag{3}$$

Assuming S and I have differing magnetic moments, they will have different Larmor frequencies when placed in an external B-field:

$$\omega_1 = -\gamma_1 \mathrm{B}_0 \tag{4}$$

$$\omega_2 = -\gamma_2 \mathrm{B}_0 \tag{5}$$

The unperturbed Hamiltonian for the system H_0, is given by:

$$H_0 = \omega_1 S_z + \omega_2 I_z \tag{6}$$

The interaction Hamiltonian $\mathcal{H}$, for this simplified quantum system is given by:

$$\mathcal{H} = \frac{\mu_0}{4\pi} \frac{\gamma_s \gamma_I}{r^3} [S \cdot I - 3(S \cdot \mathbf{n})(I \cdot \mathbf{n})] \tag{7}$$

The state space in which $\mathcal{H}$ acts is spanned by the set $\{|\varphi_{nlm}\rangle \otimes |s, i\rangle\}$,where $|\varphi_{nlm}\rangle$ is a standard basis in the state space of one of the relative particle, and $|s, i\rangle$ is the basis of eigenvectors common to S_z and I_z.

Remark 1 *The interaction Hamiltonian (dipole-dipole) of Eq. 7 neglects several terms, but for the purpose herein, i.e. the description of a quantum logic and algebra, Eq. 7 is sufficient. The reader is referred to Ref. [3] for a more complete spin Hamiltonian. As in Refs. [2]and [3], we are interested in magnetic resonance transitions of the system, since this technique allows straightforward measurement.*

The total Hamiltonian is:

$$\mathbb{H} = H_0 + \mathcal{H} \tag{8}$$

In Eq. 8 the interaction Hamiltonian term is treated as a perturbation on H_0.

Remark 2 *The transitions allowed for the spin resonance condition[2] for magnetic field parallel to the lab x-axis are:*

$$|\uparrow,\uparrow\rangle \leftrightarrow |\downarrow,\uparrow\rangle; S_x \neq 0 \tag{9}$$

$$|\uparrow,\downarrow\rangle \leftrightarrow |\downarrow,\downarrow\rangle; S_x \neq 0 \tag{10}$$

Forming a four-state quantum system with four distinct levels, depending upon which selection rule is chosen. Assume that as experimentally observed in ref. [2], that incident laser radiation can induce these spin state transitions. Then, various orientations of applied B-field and photon energy, observable spin states are forced to change in response to incident radiation (switched). Thus, we have a finite state system with four levels. The Hilbert space of possible states containing combinations of electronic and nuclear spin state vectors is finite. Additionally, undefined states are discouraged due to strict quantum mechanical selection rules and the experimental form of the perturbation (laser radiation). At some finite energy, the atom may be ionized, which would lead to loss of data. For construction of a computational machine, the energy input to the system is strictly lower than that required to ionize the atoms of the system. This energy constraint is physically realized through use of laser radiation as spin state perturbation.

Formally, if we assign to each of the four quantum levels above numeric values:

$$|\uparrow,\uparrow\rangle \Leftrightarrow 0 \tag{11}$$

$$|\uparrow,\downarrow\rangle \Leftrightarrow 1 \tag{12}$$

$$|\downarrow,\downarrow\rangle \Leftrightarrow 2 \tag{13}$$

$$|\downarrow,\uparrow\rangle \Leftrightarrow 3 \tag{14}$$

we have the basis for a four-state (finite-state) machine logic. We must now consider a transformation from physical (measurement) space to the finite group representation thereof, the elements of which, comprise the logical states of our finite state computer: the set $\mathcal{S} = \{\beta \ni \beta \in \{0,1,2,3\}\}$. Given this ordered set of elements, we write the following axioms:

Axiom 1 *All system states are subsets of S - Zorn's Lemma applies.*

Axiom 2 *Equality relation: We may write the symbol ' = ' as meaning that logical state β of the system physically corresponds to state $|\Psi\rangle$. Quantum mechanically, this implies that $|\Psi\rangle_i = |\Psi\rangle_j$, or two distinct atomic systems are physically in the same quantum state $|\Psi\rangle$. Further, if we assign the numeric value β to both states, we may say that an element is equal to itself.*

$$\beta = \beta \tag{15}$$

Axiom 3 *If two elements of S; β_i and β_j are equal, then:*

$$\beta_i = \beta_j \text{ then } \beta_j = \beta_i \tag{16}$$

Axiom 4 *There exists a transitive law:*

$$\text{If } \beta_i = \beta_j \text{ and } \beta_j = \beta_k, \text{ then } \beta_i = \beta_k \tag{17}$$

Axiom 5 *Closure. Binary operations performed upon elements of S yield elements of S.*

Remark 3

If Eqns. 11-14 are replaced by those of Eqns. 18- 21, we have a three state logic which redefines the axioms above. This tri-state logic is interesting since it can be used in the context of the radix-4 quantum computer of the present work to perform Boolean Logic, while the mappings of Eqns. 11-14 are used for arithmetical operations.

$$|\uparrow,\uparrow\rangle \Leftrightarrow 1 \tag{18}$$

$$|\uparrow,\downarrow\rangle \Leftrightarrow 0^+ \tag{19}$$

$$|\downarrow,\uparrow\rangle \Leftrightarrow 0^- \tag{20}$$

$$|\downarrow,\downarrow\rangle \Leftrightarrow -1 \tag{21}$$

Axiom 6 *All system states are subsets of S - Zorn's Lemma applies.*

Axiom 7 *Equality relation: We could only write the symbol ' = ' as meaning that logical state β of the system, which physically corresponds to $|\Psi\rangle$, is physically equal to itself IFF $\beta \in \{-1, 1\}$. Quantum mechanically, this implies that $|\Psi\rangle = |\Psi\rangle$, or is physically the same quantum state in two distinct atomic systems. However, for the zero states, 0^+ is a physically different state than 0^-. Thus we write the symbol '$\models$' for the tri-state logical equality.*

$$\beta_i \models \beta_j \tag{22}$$

Axiom 8 *Inequality ($\not\models$): If β_i is not equal to β_j, then we write:*

$$\beta_i \not\models \beta_j \tag{23}$$

We have the choice of making the logical decision that 0^+ is logically equivalent to 0^-. or:

$$0^- \models 0^+ \tag{24}$$

or

$$0^- \not\models 0^+ \tag{25}$$

If we leave this to the choosing of the programmer, then the present logic has the potential for formulation of NP complete problems. Choosing Eqn. 24 yields the tri-state logic, while choosing Eq. 25 yields a four state logic. Several tri-state logics have been discussed in the literature. [4]

4 Conclusion

The present work has presented a proposal for a simple radix-4 finite state quantum logic using quantum spin states as logic levels and photon induced spin transitions as connectives of that four state logic. A tri-state logic is seen as a special case of this four-state system. The 4-state logic is easily expandable to yet higher radix algebras and higher order quantum logics. This would be performed by exploiting material systems with larger numbers of measurable spin states. For example, doped $Bi_{12}SiO_{20}$ sillenite crystals of ref. [2] showed a rich ENDOR spin structure, including hyperfine and quadrupole lines. It is apparent that quantum mechanical spin systems offer the ability to perform calculations in higher radix than 2, and logic operations with more than two logical truth states. The present work thus proposes that the mathematics community consider multiple valued algebras and quantum logics (e.g. Quantales), while concurrently, the physics community seek to exploit the vast ESR, ENDOR, and NMR spectroscopy literature for systems capable of encoding and manipulating higher radix data.

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Chapter 4

Summary

The present report summarized the efforts of the Rome Laboratory study in Quantum Computation. The program has produced new research areas for the field as represented by two international SPIE conferences (1997,1998) chaired by Hotaling and Pirich (of Rome Laboratory) as well as providing stimulation to the community in the areas of quantum decoherence bounds in quantum computation, and representation theory for quantum groups and quantum algebras. As discussed, it is the recommendation of this study that further work be performed in quantum computation, specifically aimed at development of quantum structures and algebras to exploit the quantum gate Hamiltonians and experimental quantum computers presently in laboratories today (e.g. the ion trap and magnetic resonance systems).

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